SUPPLEMENTARY INFORMATION

DFT Calculation of NMR δ(^{113}Cd) in Cadmium Complexes.

Girolamo Casella,[a,b] Francesco Ferrante,[c] Giacomo Saielli[d,e]

[a]*Dipartimento di Scienze della Terra e del Mare (DiSTeM) dell'Università degli Studi di Palermo– Via Archirafi, 20 – 90123, Palermo, Italy*

[b] *Consorzio Interuniversitario di Ricerca in Chimica dei Metalli nei Sistemi Biologici (C.I.R.C.M.S.B.) - Piazza Umberto I, 1-70121 Bari, Italy*

[c]*Dipartimento di Fisica e Chimica dell'Università degli Studi di Palermo, Parco d' Orleans II, Viale delle Scienze, Ed. 17 - 90128, Palermo, Italy*

[d]*Dipartimento di Scienze Chimiche dell'Università, Via Marzolo, 1 - 35131 , Padova, Italy*

[e] *Istituto per la Tecnologia delle Membrane del CNR, Unità di Padova, Via Marzolo, 1 -35131, Padova, Italy*

OP2 protocol

Model 1

93

C	0.758961	1.476816	-2.567189
N	0.103165	0.457519	-2.030670
C	-0.465946	-0.231386	-3.081456
C	-0.139946	0.388841	-4.262315
N	0.641522	1.478212	-3.919346
Cd	-0.042202	0.003811	0.304094
O	-1.842073	-1.294593	-0.240883
C	-3.003383	-0.832814	-0.448363
C	-3.619951	0.427006	-0.094654
C	-4.956083	0.343662	-0.646078
N	-5.161001	-0.803825	-1.248219
N	-3.996744	-1.545297	-1.107505
C	-2.954111	1.488239	0.584844
C	-3.730789	2.608016	1.224274
C	-4.795376	2.351313	2.101779
C	-5.430288	3.401639	2.771349
C	-5.019392	4.720216	2.556547
C	-3.953421	4.983535	1.688347
C	-3.300365	3.932829	1.042769
C	-3.941794	-2.836277	-1.688545
C	-6.049893	1.368381	-0.708924
C	1.233596	2.443881	-4.831420
O	1.852588	1.311068	0.394928
C	2.991828	0.881846	0.047024
C	3.551175	-0.449926	-0.000652
C	4.889039	-0.265597	-0.521261
N	5.146117	0.999051	-0.761249
N	4.017958	1.714454	-0.386715
C	2.828884	-1.634076	0.330756
O	1.569595	-1.693447	0.426652
C	4.004117	3.115228	-0.590144
C	5.933463	-1.274419	-0.897827
C	3.544751	-2.923915	0.627375
C	3.039516	-4.123695	0.098376
C	3.635376	-5.344089	0.419074
C	4.718724	-5.385383	1.304704
C	5.205170	-4.199792	1.863211
C	4.626741	-2.974135	1.520084
N	-0.177392	-0.403625	2.633423
C	0.288335	-1.486280	3.237814
N	0.017241	-1.458778	4.568280
C	-0.664583	-0.280836	4.821502
C	-0.777863	0.359599	3.612248
C	0.369521	-2.480335	5.540392
O	-1.700084	1.570640	0.728501
H	1.322758	2.223504	-2.014047
H	-0.386133	0.160929	-5.294859
H	-1.067250	-1.120152	-2.914392
H	1.826235	3.163935	-4.252443
H	1.895733	1.937835	-5.550100
H	0.451059	2.986507	-5.383594
H	-1.246468	1.309534	3.372535
H	-0.997944	-0.014566	5.819843
H	0.820479	-2.294137	2.741843
H	1.005298	-2.057081	6.332895
H	-0.535183	-2.910220	5.996929
H	0.923624	-3.280229	5.032259
H	-6.803671	1.029603	-1.433362
H	-6.544740	1.514686	0.263232
H	-5.664993	2.351482	-1.021732
H	-5.109311	1.320201	2.276540
H	-6.248325	3.188438	3.463585
H	-5.522970	5.542054	3.071107
H	-3.623686	6.012146	1.523818
H	-2.448342	4.125865	0.388673
H	6.699301	-0.774381	-1.507123
H	6.426352	-1.716616	-0.018601
H	5.500987	-2.107227	-1.473866
H	4.999483	-2.048455	1.963336
H	6.038556	-4.228251	2.569248
H	5.178395	-6.342111	1.563818
H	3.248524	-6.269043	-0.015168
H	2.175883	-4.083499	-0.567564
C	-2.843229	-3.694237	-1.491805
C	-2.840555	-4.958456	-2.087853
C	-3.911129	-5.390086	-2.874312
C	-5.001739	-4.534475	-3.060770
C	-5.024223	-3.268311	-2.477364
H	-2.009713	-3.363708	-0.878335
H	-1.981711	-5.614881	-1.926035
H	-3.898276	-6.380694	-3.334219
H	-5.850986	-4.853612	-3.670220
H	-5.869300	-2.596902	-2.614355
C	2.982386	3.930319	-0.066250
C	3.010643	5.308178	-0.301100
C	4.039438	5.894387	-1.042356
C	5.056977	5.080010	-1.550828
C	5.046066	3.702709	-1.332257
H	2.184616	3.480406	0.518785
H	2.212989	5.929284	0.114107
H	4.053066	6.972534	-1.216400
H	5.874925	5.520220	-2.126744
H	5.836276	3.061560	-1.717953

Model 2

79

Cd	**0.066494**	**0.142531**	**0.049576**
C	**-4.539236**	**-0.976817**	**2.137305**
C	**-4.387957**	**-0.918138**	**0.741656**
C	**-5.244999**	**-1.679107**	**-0.068194**
C	**-6.247591**	**-2.467829**	**0.504795**
C	**-6.414258**	**-2.491140**	**1.892416**
C	**-5.557930**	**-1.741514**	**2.707596**
C	**-3.225449**	**-0.155048**	**0.161138**
C	**-3.396647**	**0.717212**	**-0.949677**
C	**-2.305886**	**1.231051**	**-1.757908**
N	**-2.918421**	**1.999121**	**-2.714165**
N	**-4.285769**	**2.080494**	**-2.559408**
C	**-4.583915**	**1.319454**	**-1.527482**
O	**-1.043506**	**1.085169**	**-1.716462**
C	**-2.268681**	**2.687837**	**-3.801939**
C	**-6.014280**	**1.284430**	**-1.074270**
O	**-2.115497**	**-0.388657**	**0.722617**
N	**0.022751**	**-2.091460**	**-0.777513**
C	**-0.836252**	**-3.018885**	**-0.384784**
N	**-0.580394**	**-4.210371**	**-0.985753**
C	**0.514455**	**-4.022743**	**-1.812099**
C	**0.875374**	**-2.705254**	**-1.669674**
C	**-1.311870**	**-5.449941**	**-0.785862**
O	**2.218210**	**0.205179**	**-0.808929**
C	**3.324647**	**-0.062213**	**-0.253927**
C	**4.476477**	**-0.220065**	**-1.212126**
C	**5.295543**	**-1.359218**	**-1.193847**
C	**6.287002**	**-1.535725**	**-2.163929**
C	**6.480389**	**-0.567595**	**-3.153239**
C	**5.662092**	**0.567680**	**-3.183108**
C	**4.654467**	**0.729959**	**-2.231463**
C	**3.501053**	**-0.235904**	**1.146630**
C	**2.411949**	**-0.393120**	**2.093959**
N	**3.028996**	**-0.529866**	**3.309402**
N	**4.400714**	**-0.412648**	**3.244265**
C	**4.695224**	**-0.250405**	**1.971680**
O	**1.146504**	**-0.430058**	**1.971745**
C	**6.133105**	**-0.014987**	**1.612266**
C	**2.378440**	**-0.739161**	**4.579178**
N	**0.061550**	**2.364721**	**0.936264**
C	**0.381844**	**2.780860**	**2.210390**
C	**0.247960**	**4.145158**	**2.292573**
N	**-0.161435**	**4.564752**	**1.038628**
C	**-0.259206**	**3.455849**	**0.259311**
C	**-0.439887**	**5.932135**	**0.632936**
H	**-0.565414**	**3.474575**	**-0.783050**
H	**0.402925**	**4.844698**	**3.108370**
H	**0.685736**	**2.068101**	**2.970792**
H	**-0.742103**	**5.936948**	**-0.422400**
H	**-1.256935**	**6.356925**	**1.235958**
H	**0.456053**	**6.561161**	**0.748221**
H	**1.683924**	**-2.154081**	**-2.141324**
H	**0.923883**	**-4.829092**	**-2.412919**
H	**-1.645229**	**-2.857312**	**0.323323**
H	**-1.706033**	**-5.824627**	**-1.742795**
H	**-0.662014**	**-6.218800**	**-0.340060**
H	**-2.154097**	**-5.261420**	**-0.107353**
H	**1.297920**	**-0.794211**	**4.393026**
H	**2.722375**	**-1.678664**	**5.041867**
H	**2.596683**	**0.090225**	**5.272427**
H	**6.697212**	**0.161397**	**2.539178**
H	**6.586543**	**-0.872030**	**1.090739**
H	**6.248863**	**0.857293**	**0.949751**
H	**5.137108**	**-2.120011**	**-0.426896**
H	**6.909271**	**-2.433818**	**-2.147044**
H	**7.261583**	**-0.700561**	**-3.905563**
H	**5.803985**	**1.323369**	**-3.959574**
H	**3.990528**	**1.595410**	**-2.266702**
H	**-2.661214**	**2.339247**	**-4.770979**
H	**-2.432938**	**3.776571**	**-3.733728**
H	**-1.194914**	**2.467286**	**-3.740023**
H	**-6.562307**	**2.083393**	**-1.593702**
H	**-6.508391**	**0.326673**	**-1.299748**
H	**-6.099806**	**1.437906**	**0.013009**
H	**-5.109345**	**-1.665498**	**-1.151536**
H	**-6.901290**	**-3.065041**	**-0.135660**
H	**-7.205204**	**-3.097979**	**2.339680**
H	**-5.679685**	**-1.762225**	**3.793290**
H	**-3.846879**	**-0.414414**	**2.766160**

Model 3

113

Cd	**0.269041**	**0.049400**	**-0.072127**
C	**3.455303**	**0.331846**	**-1.257141**
N	**2.623694**	**-0.155922**	**-0.268898**
C	**3.399433**	**-0.769648**	**0.607095**
N	**4.710986**	**-0.704893**	**0.231838**
C	**4.753189**	**0.003735**	**-0.963715**
O	**0.579039**	**-1.641092**	**1.518609**
C	**0.293116**	**-2.871537**	**1.464058**
C	**0.817256**	**-3.691629**	**2.611231**
C	**0.722425**	**-3.181217**	**3.917053**
C	**1.272131**	**-3.881617**	**4.991429**
C	**1.958131**	**-5.081642**	**4.770380**
C	**2.086902**	**-5.579527**	**3.470341**
C	**1.512166**	**-4.892524**	**2.396494**
C	**5.829953**	**-1.256698**	**0.950883**
O	**-0.241538**	**-1.769062**	**-1.386772**
C	**-0.636209**	**-2.868451**	**-0.897426**
N	**-1.404411**	**-3.785459**	**-1.606552**
N	**-1.752899**	**-4.882254**	**-0.830960**
C	**-1.175160**	**-4.719304**	**0.336484**
C	**-0.435030**	**-3.477409**	**0.397622**
C	**-1.913057**	**-3.698726**	**-2.925154**
C	**-2.865815**	**-4.646107**	**-3.346642**
C	**-3.384826**	**-4.586246**	**-4.640088**
C	**-2.972209**	**-3.591167**	**-5.532474**
C	**-2.022407**	**-2.657386**	**-5.111965**
C	**-1.486162**	**-2.700433**	**-3.821800**
C	**-1.446321**	**-5.742766**	**1.399404**
O	**0.509333**	**1.698107**	**-1.678236**
C	**0.529602**	**2.957243**	**-1.549910**
C	**0.214833**	**3.649815**	**-0.345061**
C	**0.129136**	**3.029607**	**0.958856**
N	**-0.213064**	**4.059669**	**1.824353**
N	**-0.410357**	**5.257680**	**1.152932**
C	**-0.147825**	**5.032306**	**-0.112480**
O	**0.319854**	**1.836824**	**1.342243**
C	**-0.354402**	**6.160946**	**-1.078828**
C	**-0.446135**	**4.019696**	**3.221370**
C	**-0.168958**	**2.872624**	**3.988892**
C	**-0.417538**	**2.886770**	**5.364168**
C	**-0.933453**	**4.021297**	**5.994657**
C	**-1.201055**	**5.159214**	**5.226684**
C	**-0.962937**	**5.166199**	**3.852926**
N	**-2.109494**	**0.210955**	**0.121080**
C	**-2.973769**	**-0.290562**	**-0.744857**
N	**-4.259183**	**-0.068476**	**-0.343695**
C	**-4.191066**	**0.624957**	**0.858525**
C	**-2.857202**	**0.786746**	**1.129460**
C	**-5.449106**	**-0.477389**	**-1.044034**
C	**0.950667**	**3.704070**	**-2.786784**
C	**1.974441**	**4.663192**	**-2.747425**
C	**2.427827**	**5.263224**	**-3.925870**
C	**1.850615**	**4.923541**	**-5.152727**
C	**0.833604**	**3.962912**	**-5.200626**
C	**0.400797**	**3.342717**	**-4.027896**
H	**-2.715349**	**-0.795269**	**-1.670995**
H	**-5.082666**	**0.900322**	**1.411085**
H	**-2.384183**	**1.271281**	**1.978542**
H	**3.054529**	**0.878066**	**-2.105936**
H	**5.683047**	**0.169119**	**-1.496802**
H	**3.051245**	**-1.243353**	**1.520259**
H	**-0.875610**	**6.975588**	**-0.556858**
H	**0.593738**	**6.553840**	**-1.476015**
H	**-0.956447**	**5.844929**	**-1.945063**
H	**2.431310**	**4.920575**	**-1.789667**
H	**3.235617**	**5.997798**	**-3.885025**
H	**2.197694**	**5.400467**	**-6.072410**
H	**0.384565**	**3.689208**	**-6.158334**
H	**-0.369994**	**2.570771**	**-4.058942**
H	**-2.264948**	**-6.392220**	**1.059200**
H	**-0.568959**	**-6.373380**	**1.608553**
H	**-1.733869**	**-5.269361**	**2.351081**
H	**1.618859**	**-5.275312**	**1.379471**
H	**2.635769**	**-6.506996**	**3.290329**
H	**2.397385**	**-5.624241**	**5.610829**
H	**1.174557**	**-3.486495**	**6.005304**
H	**0.211116**	**-2.230242**	**4.075250**
H	**0.236793**	**1.989552**	**3.503211**
H	**-0.196460**	**1.989762**	**5.948285**
H	**-1.122217**	**4.021110**	**7.070440**
H	**-1.602190**	**6.058578**	**5.700701**
H	**-1.165718**	**6.047469**	**3.247932**
H	**-0.740053**	**-1.977076**	**-3.503647**
H	**-1.680424**	**-1.878573**	**-5.798048**
H	**-3.381888**	**-3.548894**	**-6.543927**
H	**-4.119460**	**-5.332669**	**-4.952779**
H	**-3.172282**	**-5.422758**	**-2.648656**
C	**7.054817**	**-0.977893**	**0.226677**
H	**5.883054**	**-0.806216**	**1.940917**
H	**5.703153**	**-2.333873**	**1.048531**
C	**-6.618373**	**-0.056293**	**-0.297045**
H	**-5.464728**	**-0.018791**	**-2.031639**
H	**-5.455203**	**-1.561486**	**-1.147074**
C	**8.070942**	**-0.228909**	**0.832080**
C	**9.253571**	**0.040281**	**0.132846**
C	**9.420073**	**-0.439512**	**-1.171790**
C	**8.403948**	**-1.188496**	**-1.777193**
C	**7.221319**	**-1.457686**	**-1.077959**
H	**7.941427**	**0.144301**	**1.846901**
H	**10.043971**	**0.622884**	**0.603763**
H	**10.339989**	**-0.230121**	**-1.715694**
H	**8.533463**	**-1.561707**	**-2.792013**
H	**6.430919**	**-2.040289**	**-1.548876**
C	**-7.546962**	**0.813035**	**-0.881845**
C	**-8.675910**	**1.219610**	**-0.160614**
C	**-8.876268**	**0.756859**	**1.145417**
C	**-7.947678**	**-0.112469**	**1.730217**
C	**-6.818731**	**-0.519044**	**1.008986**
H	**-7.391112**	**1.172989**	**-1.897751**
H	**-9.398220**	**1.895823**	**-0.615505**
H	**-9.754428**	**1.073117**	**1.706432**
H	**-8.103528**	**-0.472423**	**2.746123**
H	**-6.096422**	**-1.195256**	**1.463878**

Model 4

99

Cd	**0.142493**	**-0.426020**	**0.112555**
C	**4.207441**	**-2.606401**	**1.994412**
C	**4.411181**	**-3.399450**	**0.849473**
C	**5.594067**	**-4.152747**	**0.731468**
C	**6.555051**	**-4.106911**	**1.740717**
C	**6.361960**	**-3.316449**	**2.878330**
C	**5.184874**	**-2.573272**	**2.992926**
N	**3.454949**	**-3.469001**	**-0.194533**
C	**2.312401**	**-2.704252**	**-0.396200**
C	**1.757874**	**-3.181283**	**-1.641448**
C	**2.668409**	**-4.221912**	**-2.065683**
N	**3.656759**	**-4.382404**	**-1.217922**
O	**1.946506**	**-1.791898**	**0.405667**
O	**-0.145182**	**-1.762963**	**-1.779061**
C	**0.570015**	**-2.686232**	**-2.256621**
C	**0.087672**	**-3.277790**	**-3.572155**
C	**2.643621**	**-5.106343**	**-3.276393**
N	**1.697109**	**1.065590**	**-0.878828**
C	**3.013774**	**0.954435**	**-0.793895**
N	**3.633958**	**1.992437**	**-1.414633**
C	**2.642555**	**2.813375**	**-1.925700**
C	**1.450329**	**2.225118**	**-1.583675**
O	**0.174623**	**0.718719**	**2.117592**
C	**-0.544840**	**1.661259**	**2.546307**
C	**-1.607217**	**2.263721**	**1.807007**
C	**-1.973980**	**1.928172**	**0.451194**
N	**-3.074262**	**2.731392**	**0.167226**
N	**-3.414747**	**3.544324**	**1.237906**
C	**-2.558841**	**3.280127**	**2.196752**
O	**-1.476711**	**1.120790**	**-0.389386**
C	**-2.704822**	**4.036480**	**3.483256**
C	**-3.873901**	**2.780336**	**-0.999481**
C	**-3.574251**	**2.015581**	**-2.143747**
C	**-4.403770**	**2.097651**	**-3.265891**
C	**-5.527529**	**2.927252**	**-3.277455**
C	**-5.818055**	**3.686822**	**-2.138978**
C	**-5.005303**	**3.618924**	**-1.007508**
N	**-1.585242**	**-1.796982**	**1.016559**
C	**-2.100571**	**-1.876768**	**2.293308**
C	**-3.338618**	**-2.468490**	**2.252248**
N	**-3.579645**	**-2.755290**	**0.919831**
C	**-2.497534**	**-2.329615**	**0.217926**
C	**-0.221289**	**2.144136**	**3.951745**
H	**3.541412**	**0.144106**	**-0.297193**
H	**2.876031**	**3.726706**	**-2.463414**
H	**0.434345**	**2.549739**	**-1.788418**
H	**-1.546456**	**-1.504048**	**3.149732**
H	**-4.061302**	**-2.700706**	**3.027989**
H	**-2.404293**	**-2.412899**	**-0.861849**
H	**-3.556054**	**4.724739**	**3.389435**
H	**-2.891423**	**3.366610**	**4.338234**
H	**-1.804654**	**4.625860**	**3.720780**
H	**3.511755**	**-5.778456**	**-3.235426**
H	**1.729991**	**-5.720749**	**-3.321712**
H	**2.694815**	**-4.528197**	**-4.213273**
H	**-2.699684**	**1.371105**	**-2.140723**
H	**-4.157316**	**1.499290**	**-4.146739**
H	**-6.166655**	**2.984863**	**-4.161234**
H	**-6.689534**	**4.346438**	**-2.127762**
H	**-5.222509**	**4.207413**	**-0.118537**
H	**3.291458**	**-2.030512**	**2.091227**
H	**5.012242**	**-1.955182**	**3.877662**
H	**7.117933**	**-3.284095**	**3.665994**
H	**7.467208**	**-4.699204**	**1.632979**
H	**5.733646**	**-4.768258**	**-0.154845**
H	**-0.818041**	**-2.741376**	**-3.882423**
H	**0.851326**	**-3.180187**	**-4.358670**
H	**-0.139912**	**-4.350403**	**-3.469237**
H	**-1.076298**	**2.000068**	**4.630389**
H	**0.635959**	**1.569982**	**4.325285**
H	**0.025646**	**3.216936**	**3.960445**
C	**5.079870**	**2.188742**	**-1.533598**
H	**5.551813**	**1.310397**	**-1.067725**
H	**5.353250**	**2.177079**	**-2.599866**
C	**5.573215**	**3.468297**	**-0.885306**
C	**6.301581**	**4.402965**	**-1.631423**
C	**6.781953**	**5.573225**	**-1.033766**
C	**6.532423**	**5.820141**	**0.317612**
C	**5.802550**	**4.892101**	**1.069485**
C	**5.327235**	**3.723759**	**0.472756**
H	**6.497845**	**4.214610**	**-2.690594**
H	**7.348777**	**6.293117**	**-1.628360**
H	**6.904099**	**6.734002**	**0.786336**
H	**5.604241**	**5.079648**	**2.127124**
H	**4.755134**	**3.005260**	**1.065296**
C	**-4.805651**	**-3.318051**	**0.353771**
C	**-5.979417**	**-2.354390**	**0.361441**
H	**-4.561139**	**-3.623419**	**-0.675560**
H	**-5.060463**	**-4.232774**	**0.909448**
C	**-7.218606**	**-2.760859**	**0.872088**
C	**-8.315552**	**-1.893036**	**0.849824**
C	**-8.178693**	**-0.607532**	**0.321072**
C	**-6.942472**	**-0.191840**	**-0.186774**
C	**-5.850348**	**-1.061086**	**-0.168057**
H	**-7.329742**	**-3.765335**	**1.290500**
H	**-9.276221**	**-2.222773**	**1.252099**
H	**-9.032965**	**0.073084**	**0.306792**
H	**-6.822528**	**0.812285**	**-0.599009**
H	**-4.890231**	**-0.720923**	**-0.563768**

Model 5

99

Cd	-0.108541	0.266141	0.147138
C	-3.494933	0.240738	0.699262
N	-2.396789	-0.393344	0.154418
C	-2.847328	-1.485076	-0.436487
N	-4.202835	-1.593515	-0.301494
C	-4.624770	-0.485340	0.424862
O	0.181419	-1.975607	-0.555050
C	0.792382	-2.916647	0.027397
C	0.768379	-4.234958	-0.697673
C	0.956776	-4.252739	-2.090162
C	0.865516	-5.449967	-2.801023
C	0.545372	-6.639325	-2.135701
C	0.321982	-6.624978	-0.755801
C	0.440965	-5.430540	-0.038759
C	-5.028747	-2.648027	-0.830149
N	2.265126	0.689525	-0.031947
C	3.167223	0.501314	0.914474
N	4.435035	0.600507	0.420303
C	4.315432	0.878109	-0.936466
C	2.969629	0.924705	-1.195847
C	5.651374	0.421743	1.170079
O	-0.837504	2.321565	0.873106
C	-1.142303	3.357685	0.209445
C	-0.869042	3.537267	-1.173744
C	-0.441719	2.476594	-2.068713
N	-0.304710	3.086719	-3.286507
N	-0.538686	4.444716	-3.248854
C	-0.884302	4.723837	-2.010178
O	-0.222318	1.233223	-1.907437
C	-1.126230	6.162497	-1.659007
C	0.081014	2.452480	-4.522916
O	0.406637	-0.679747	2.164416
C	1.175968	-1.688937	2.211572
C	1.434467	-2.780252	1.293635
C	2.469529	-3.559134	1.940523
N	2.806871	-3.041099	3.106685
N	2.000115	-1.934851	3.281878
C	3.248194	-4.742158	1.444844
C	2.045079	-1.185696	4.514982
C	-1.867526	4.409484	1.006881
C	-3.096313	4.934777	0.579089
C	-3.806573	5.826304	1.388904
C	-3.287631	6.214555	2.627146
C	-2.066126	5.688911	3.064091
C	-1.371096	4.777282	2.268314
H	2.955989	0.307965	1.960365
H	5.185471	0.977278	-1.576595
H	2.451152	1.101119	-2.133217
H	-3.389478	1.168322	1.254591
H	-5.664104	-0.347066	0.702292
H	-2.230104	-2.195508	-0.979191
H	0.172284	1.375625	-4.329978
H	-0.681623	2.626551	-5.298896
H	1.044062	2.849116	-4.886209
H	-0.794711	6.785004	-2.502178
H	-2.188097	6.379323	-1.465620
H	-0.571905	6.458080	-0.754299
H	-3.504616	4.624086	-0.384743
H	-4.768985	6.218121	1.050894
H	-3.837476	6.919310	3.255534
H	-1.660288	5.983319	4.034945
H	-0.434239	4.337985	2.615213
H	1.759870	-1.821862	5.368734
H	3.057960	-0.790619	4.699147
H	1.333257	-0.354845	4.422456
H	4.114419	-4.893360	2.104605
H	2.652821	-5.667947	1.442215
H	3.604102	-4.590625	0.413371
H	0.255776	-5.415459	1.037131
H	0.053339	-7.546971	-0.234524
H	0.463076	-7.574658	-2.694516
H	1.034700	-5.456103	-3.880462
H	1.175710	-3.314584	-2.602847
C	-6.412551	-2.403410	-0.472732
H	-4.933228	-2.674864	-1.914619
H	-4.709574	-3.602381	-0.413904
C	-7.376892	-2.244695	-1.475158
C	-8.712980	-2.008514	-1.130068
C	-9.084727	-1.931048	0.217450
C	-8.120387	-2.089763	1.219876
C	-6.784299	-2.325944	0.874785
H	-7.087725	-2.304954	-2.523334
H	-9.463098	-1.885056	-1.909812
H	-10.124013	-1.747332	0.485882
H	-8.409554	-2.029505	2.268052
H	-6.034181	-2.449402	1.654529
C	6.791293	0.607693	0.293435
H	5.691051	1.151984	1.976983
H	5.675431	-0.583342	1.588583
C	7.725448	1.614763	0.563926
C	8.826060	1.794300	-0.282489
C	8.992518	0.966767	-1.399397
C	8.058364	-0.040304	-1.669887
C	6.957752	-0.219841	-0.823473
H	7.595966	2.258465	1.432720
H	9.552698	2.577656	-0.072086
H	9.848638	1.106421	-2.057786
H	8.187844	-0.684006	-2.538682
H	6.231113	-1.003198	-1.033876

Model 6

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Cd	**0.000211**	**-0.000211**	**0.000516**
C	**-2.818382**	**2.734498**	**-2.478482**
C	**-1.508765**	**2.347349**	**-2.124415**
N	**-1.560997**	**1.351853**	**-1.220076**
N	**-2.875200**	**1.090039**	**-0.984276**
C	**-3.648798**	**1.910356**	**-1.731181**
N	**1.559781**	**-1.353108**	**1.221668**
N	**2.874076**	**-1.089964**	**0.986846**
C	**3.647768**	**-1.908964**	**1.735118**
C	**2.817591**	**-2.733548**	**2.482118**
C	**1.507926**	**-2.347889**	**2.126609**
B	**-3.356606**	**-0.002704**	**0.007273**
N	**-2.866972**	**0.309494**	**1.446224**
N	**-1.551345**	**0.381157**	**1.786287**
C	**-1.494009**	**0.667852**	**3.100020**
C	**-2.801626**	**0.784067**	**3.616700**
C	**-3.636237**	**0.548894**	**2.532652**
B	**3.356604**	**0.001297**	**-0.005315**
N	**2.871586**	**1.405202**	**0.444637**
N	**1.556688**	**1.736317**	**0.558978**
C	**1.502082**	**3.018456**	**0.964516**
C	**2.810732**	**3.523766**	**1.114367**
C	**3.643099**	**2.466107**	**0.774094**
N	**-1.556565**	**-1.736838**	**-0.557972**
N	**-2.871594**	**-1.405446**	**-0.445295**
C	**-3.642934**	**-2.463860**	**-0.782891**
C	**-2.810456**	**-3.520279**	**-1.126614**
C	**-1.501862**	**-3.016706**	**-0.970420**
N	**1.552438**	**-0.381280**	**-1.784337**
N	**2.868183**	**-0.311610**	**-1.444624**
C	**3.636928**	**-0.552013**	**-2.531098**
C	**2.801745**	**-0.785587**	**-3.615102**
C	**1.494362**	**-0.667737**	**-3.098238**
H	**-4.567638**	**-0.004016**	**0.011649**
H	**4.567650**	**0.001795**	**-0.008487**
C	**0.210654**	**-2.907725**	**2.630284**
H	**4.731137**	**-1.845552**	**1.681521**
H	**3.109664**	**-3.507193**	**3.186700**
H	**-4.726474**	**-2.388422**	**-0.753725**
H	**-3.100472**	**-4.517298**	**-1.446178**
C	**-0.203017**	**-3.728923**	**-1.206479**
C	**0.194458**	**-0.822507**	**-3.830380**
H	**3.089408**	**-1.009733**	**-4.638484**
H	**4.720651**	**-0.538829**	**-2.453924**
C	**0.203318**	**3.730697**	**1.201128**
H	**3.100851**	**4.522461**	**1.428569**
H	**4.726607**	**2.391084**	**0.742988**
C	**-0.194223**	**0.822105**	**3.832556**
H	**-3.089741**	**1.008212**	**4.639940**
H	**-4.719922**	**0.534499**	**2.455285**
C	**-0.211694**	**2.907936**	**-2.627686**
H	**-3.110321**	**3.508607**	**-3.182629**
H	**-4.732163**	**1.847718**	**-1.676694**
H	**-0.381262**	**1.062759**	**4.888974**
H	**0.408957**	**-0.097701**	**3.791780**
H	**0.424938**	**1.623574**	**3.401767**
H	**0.391229**	**4.769959**	**1.507050**
H	**-0.424398**	**3.745806**	**0.297256**
H	**-0.392014**	**3.244113**	**1.988842**
H	**-0.402503**	**3.698581**	**-3.367604**
H	**0.390382**	**3.338738**	**-1.813184**
H	**0.410880**	**2.134986**	**-3.103256**
H	**-0.390405**	**-4.772372**	**-1.498146**
H	**0.386194**	**-3.251312**	**-2.004385**
H	**0.430335**	**-3.730674**	**-0.306617**
H	**0.381453**	**-1.041213**	**-4.891573**
H	**-0.414420**	**-1.639377**	**-3.413815**
H	**-0.419151**	**0.089073**	**-3.770318**
H	**0.401105**	**-3.711197**	**3.356318**
H	**-0.402814**	**-2.138030**	**3.122973**
H	**-0.400388**	**-3.320664**	**1.813372**

Model 7

91

Cd	**-0.000092**	**-0.001481**	**-0.032886**
C	**2.938706**	**3.507415**	**-0.224016**
C	**1.621896**	**3.027851**	**-0.064465**
N	**1.633260**	**1.685106**	**-0.032015**
N	**2.929174**	**1.281480**	**-0.173869**
C	**3.729817**	**2.372809**	**-0.284030**
N	**-1.634757**	**-1.683967**	**-0.077485**
N	**-2.930876**	**-1.275919**	**-0.203837**
C	**-3.733551**	**-2.363938**	**-0.331304**
C	**-2.943483**	**-3.500402**	**-0.299070**
C	**-1.625184**	**-3.025569**	**-0.137479**
B	**3.400076**	**-0.212697**	**-0.065205**
N	**2.799485**	**-1.081666**	**-1.220382**
N	**1.535388**	**-0.895474**	**-1.699448**
C	**1.310596**	**-1.858524**	**-2.610521**
C	**2.442098**	**-2.696279**	**-2.710532**
C	**3.351293**	**-2.176670**	**-1.803286**
B	**-3.400099**	**0.215899**	**-0.059979**
N	**-2.797999**	**1.111947**	**-1.193567**
N	**-1.533020**	**0.938035**	**-1.674839**
C	**-1.307331**	**1.922545**	**-2.562453**
C	**-2.439359**	**2.761485**	**-2.644680**
C	**-3.349718**	**2.219952**	**-1.751563**
N	**1.572034**	**-1.019828**	**1.476528**
N	**2.913579**	**-0.819685**	**1.287960**
C	**3.597529**	**-1.269264**	**2.369670**
C	**2.685804**	**-1.772805**	**3.283605**
C	**1.422885**	**-1.593109**	**2.683138**
N	**-1.571619**	**0.975674**	**1.504633**
N	**-2.913898**	**0.788776**	**1.308070**
C	**-3.597942**	**1.220497**	**2.396961**
C	**-2.685461**	**1.697953**	**3.324067**
C	**-1.421931**	**1.521244**	**2.724010**
N	**4.930213**	**-0.217508**	**-0.221268**
N	**-4.930009**	**0.226196**	**-0.217059**
C	**-0.358578**	**-3.819432**	**-0.041858**
H	**-4.809886**	**-2.260678**	**-0.420222**
H	**-3.272029**	**-4.533248**	**-0.372783**
H	**4.676755**	**-1.170037**	**2.397991**
H	**2.901503**	**-2.209127**	**4.254962**
C	**0.078812**	**-1.969073**	**3.228500**
C	**-0.075508**	**1.861932**	**3.286280**
H	**-2.901186**	**2.115647**	**4.303576**
H	**-4.678003**	**1.129405**	**2.419818**
C	**-0.019456**	**2.018633**	**-3.322375**
H	**-2.574881**	**3.637279**	**-3.273276**
H	**-4.351135**	**2.541656**	**-1.483326**
C	**0.024156**	**-1.935484**	**-3.375114**
H	**2.578168**	**-3.557008**	**-3.359492**
H	**4.352029**	**-2.505415**	**-1.541080**
C	**0.355552**	**3.818514**	**0.057173**
H	**3.265724**	**4.541961**	**-0.278111**
H	**4.805708**	**2.272706**	**-0.381551**
N	**5.766001**	**-0.025212**	**0.841153**
C	**6.982128**	**0.186457**	**0.337402**
C	**6.947610**	**0.161230**	**-1.082271**
C	**5.626205**	**-0.088479**	**-1.394225**
H	**5.132039**	**-0.167617**	**-2.357934**
H	**7.772132**	**0.299245**	**-1.776885**
C	**8.158118**	**0.399019**	**1.241682**
C	**-5.624574**	**0.122494**	**-1.393382**
C	**-6.946765**	**-0.131554**	**-1.088454**
C	**-6.983262**	**-0.186139**	**0.330352**
N	**-5.767527**	**0.013274**	**0.840067**
C	**-8.160868**	**-0.415640**	**1.228377**
H	**-7.770525**	**-0.253991**	**-1.786883**
H	**-5.128885**	**0.220744**	**-2.354560**
H	**0.130730**	**1.278158**	**4.198344**
H	**0.726162**	**1.658975**	**2.564918**
H	**-0.028080**	**2.927154**	**3.565800**
H	**0.415351**	**3.027489**	**-3.239124**
H	**0.714837**	**1.293586**	**-2.948117**
H	**-0.184472**	**1.823089**	**-4.395460**
H	**-0.471885**	**-4.641947**	**0.682284**
H	**-0.097033**	**-4.272377**	**-1.012273**
H	**0.484439**	**-3.191457**	**0.273921**
H	**-0.414270**	**-2.944292**	**-3.312666**
H	**-0.708734**	**-1.215529**	**-2.988478**
H	**0.192513**	**-1.719602**	**-4.443754**
H	**-0.074180**	**-1.535232**	**4.229784**
H	**-0.733350**	**-1.623290**	**2.576654**
H	**-0.008821**	**-3.063415**	**3.333459**
H	**0.469177**	**4.616910**	**0.807870**
H	**0.094144**	**4.302939**	**-0.897918**
H	**-0.487422**	**3.181039**	**0.353205**
H	**-7.826280**	**-0.520726**	**2.270056**
H	**-8.875710**	**0.423342**	**1.179052**
H	**-8.710330**	**-1.328205**	**0.944672**
H	**8.705280**	**1.319340**	**0.979361**
H	**7.822109**	**0.479539**	**2.285093**
H	**8.875444**	**-0.436568**	**1.174200**

Model 8

53

Cd	**0.002026**	**-0.001099**	**0.000085**
Br	**-0.349291**	**-5.714407**	**2.851333**
Br	**4.910350**	**-2.332095**	**-3.370198**
Br	**4.897968**	**2.232166**	**3.451887**
Br	**-4.643591**	**2.788751**	**3.390989**
Br	**-4.639542**	**-2.693634**	**-3.470689**
Br	**-0.181964**	**5.720617**	**-2.853641**
C	**-0.114608**	**3.864766**	**-2.514669**
C	**-0.105728**	**3.222735**	**-1.264503**
N	**-0.054530**	**1.897028**	**-1.439571**
N	**-0.030389**	**1.667048**	**-2.777541**
C	**-0.064450**	**2.840774**	**-3.452347**
N	**-0.120667**	**-1.895606**	**1.438221**
N	**-0.113431**	**-1.665825**	**2.776482**
C	**-0.186169**	**-2.838103**	**3.450761**
C	**-0.239293**	**-3.861336**	**2.512594**
C	**-0.192113**	**-3.220404**	**1.262643**
B	**0.030323**	**0.235110**	**-3.377179**
N	**-1.218164**	**-0.580252**	**-2.941580**
N	**-1.499126**	**-0.846062**	**-1.640000**
C	**-2.629572**	**-1.561853**	**-1.615117**
C	**-3.093108**	**-1.759339**	**-2.927099**
C	**-2.166873**	**-1.121172**	**-3.742523**
B	**-0.032763**	**-0.235786**	**3.377533**
N	**-1.256331**	**0.606119**	**2.921381**
N	**-1.509084**	**0.877627**	**1.615197**
C	**-2.624569**	**1.615544**	**1.570902**
C	**-3.105152**	**1.825000**	**2.874937**
C	**-2.205193**	**1.169719**	**3.706162**
N	**1.604810**	**-0.720226**	**-1.607239**
N	**1.328049**	**-0.483548**	**-2.915283**
C	**2.329006**	**-0.955432**	**-3.695855**
C	**3.286636**	**-1.516425**	**-2.860106**
C	**2.786446**	**-1.346475**	**-1.557710**
N	**1.589477**	**0.687953**	**1.633792**
N	**1.287062**	**0.455613**	**2.936865**
C	**2.286146**	**0.903752**	**3.733734**
C	**3.266257**	**1.449941**	**2.914351**
C	**2.783812**	**1.290701**	**1.603941**
H	**0.039758**	**0.317245**	**-4.582470**
H	**-0.045039**	**-0.318560**	**4.582817**
H	**-0.209325**	**-3.652264**	**0.265013**
H	**-0.195794**	**-2.870808**	**4.535793**
H	**2.298599**	**-0.863350**	**-4.777065**
H	**3.222953**	**-1.643496**	**-0.607340**
H	**3.240893**	**1.579503**	**0.660679**
H	**2.238576**	**0.808312**	**4.814051**
H	**-3.031636**	**1.957980**	**0.622709**
H	**-2.182898**	**1.069010**	**4.786804**
H	**-3.057832**	**-1.898650**	**-0.674265**
H	**-2.124977**	**-1.019927**	**-4.822542**
H	**-0.135110**	**3.654720**	**-0.267168**
H	**-0.053315**	**2.874033**	**-4.537345**

Model 9

71

Cd	**-0.000171**	**0.000104**	**-0.005001**
C	**2.771987**	**3.699617**	**-0.337696**
C	**1.486171**	**3.119344**	**-0.294683**
N	**1.562674**	**1.788473**	**-0.170996**
N	**2.879885**	**1.472368**	**-0.131738**
C	**3.622429**	**2.602989**	**-0.230409**
N	**-1.562668**	**-1.792844**	**-0.109125**
N	**-2.879903**	**-1.475703**	**-0.080459**
C	**-3.622337**	**-2.609073**	**-0.140827**
C	**-2.771798**	**-3.708616**	**-0.211369**
C	**-1.486039**	**-3.127107**	**-0.188342**
B	**3.383879**	**0.009852**	**0.003458**
N	**2.891518**	**-0.840909**	**-1.198849**
N	**1.576758**	**-1.035884**	**-1.462919**
C	**1.510214**	**-1.806621**	**-2.555407**
C	**2.800329**	**-2.131803**	**-3.026404**
C	**3.642579**	**-1.489554**	**-2.123348**
B	**-3.383909**	**-0.009408**	**0.004239**
N	**-2.891672**	**0.799397**	**-1.226689**
N	**-1.576933**	**0.985403**	**-1.497385**
C	**-1.510594**	**1.718229**	**-2.615685**
C	**-2.800785**	**2.026871**	**-3.097452**
C	**-3.642873**	**1.415899**	**-2.172797**
N	**1.568251**	**-0.744652**	**1.627721**
N	**2.884684**	**-0.608008**	**1.337375**
C	**3.629596**	**-1.083970**	**2.366070**
C	**2.781175**	**-1.549558**	**3.366497**
C	**1.494204**	**-1.307569**	**2.840059**
N	**-1.568059**	**0.800782**	**1.601142**
N	**-2.884579**	**0.654007**	**1.316116**
C	**-3.629208**	**1.163578**	**2.328778**
C	**-2.780519**	**1.662851**	**3.312608**
C	**-1.493689**	**1.404058**	**2.793894**
H	**4.594815**	**0.015302**	**0.006096**
H	**-4.594847**	**-0.014778**	**0.007159**
H	**-0.510645**	**-3.610038**	**-0.225837**
H	**-4.708390**	**-2.558807**	**-0.130218**
C	**-3.139522**	**-5.161262**	**-0.292321**
H	**4.715601**	**-1.060003**	**2.318878**
C	**3.151462**	**-2.161071**	**4.685916**
H	**0.519429**	**-1.512982**	**3.280062**
H	**-0.518796**	**1.624597**	**3.226237**
C	**-3.150538**	**2.317716**	**4.611134**
H	**-4.715228**	**1.137535**	**2.282969**
H	**-0.538669**	**1.992257**	**-3.023473**
C	**-3.179174**	**2.819688**	**-4.314100**
H	**-4.728503**	**1.379908**	**-2.125551**
H	**0.538237**	**-2.094335**	**-2.953531**
C	**3.178398**	**-2.966057**	**-4.215125**
H	**4.728213**	**-1.452093**	**-2.077437**
H	**0.510842**	**3.600907**	**-0.348110**
C	**3.139725**	**5.148701**	**-0.467554**
H	**4.708474**	**2.552937**	**-0.218387**
H	**4.271789**	**-3.055086**	**-4.303779**
H	**2.768636**	**-3.987823**	**-4.146483**
H	**2.805523**	**-2.530507**	**-5.157586**
H	**4.244381**	**-2.222304**	**4.800221**
H	**2.763657**	**-1.572704**	**5.534647**
H	**2.750982**	**-3.183483**	**4.790858**
H	**4.232450**	**5.279561**	**-0.476658**
H	**2.746960**	**5.590041**	**-1.399079**
H	**2.742363**	**5.749395**	**0.367952**
H	**-4.272600**	**2.905323**	**-4.405630**
H	**-2.769699**	**3.843326**	**-4.280685**
H	**-2.806267**	**2.352096**	**-5.241067**
H	**-4.232247**	**-5.292316**	**-0.297375**
H	**-2.746444**	**-5.633788**	**-1.208283**
H	**-2.742459**	**-5.733412**	**0.563124**
H	**-4.243441**	**2.381685**	**4.724057**
H	**-2.761629**	**1.758281**	**5.478714**
H	**-2.750974**	**3.343431**	**4.681768**

Model 10

91

Cd	**0.000098**	**-0.064428**	**0.000141**
N	**5.749541**	**0.491783**	**0.972483**
N	**4.951392**	**-0.056060**	**0.017004**
C	**5.679552**	**-0.908406**	**-0.774600**
C	**6.995264**	**-0.895615**	**-0.344486**
C	**6.968251**	**0.005304**	**0.752264**
B	**3.419474**	**0.050146**	**0.057918**
N	**2.895541**	**1.343902**	**0.759882**
N	**1.555405**	**1.585606**	**0.738847**
C	**1.363189**	**2.750882**	**1.367027**
C	**2.585390**	**3.298188**	**1.807451**
C	**3.530463**	**2.363795**	**1.397225**
N	**-1.555245**	**1.584572**	**-0.740947**
N	**-2.895476**	**1.343342**	**-0.761067**
C	**-3.530428**	**2.363340**	**-1.398234**
C	**-2.585267**	**3.297246**	**-1.809347**
C	**-1.362989**	**2.749603**	**-1.369549**
B	**-3.419416**	**0.050174**	**-0.058029**
N	**-4.951321**	**-0.056135**	**-0.017267**
N	**-5.749432**	**0.491541**	**-0.972870**
C	**-6.968146**	**0.005075**	**-0.752640**
C	**-6.995199**	**-0.895667**	**0.344256**
C	**-5.679513**	**-0.908361**	**0.774441**
N	**-1.619602**	**-0.240249**	**1.747842**
C	**-1.468344**	**0.048063**	**3.045913**
C	**-2.657946**	**0.569042**	**3.596351**
C	**-3.533535**	**0.578410**	**2.516926**
N	**-2.900144**	**0.073701**	**1.422183**
N	**1.619744**	**-0.242979**	**-1.747576**
N	**2.900014**	**0.072391**	**-1.422199**
C	**3.532760**	**0.577436**	**-2.517152**
C	**2.657045**	**0.566845**	**-3.596470**
C	**1.468043**	**0.044831**	**-3.045721**
N	**-1.566583**	**-1.461028**	**-1.029318**
N	**-2.884546**	**-1.210359**	**-0.828636**
C	**-3.623970**	**-2.145869**	**-1.485538**
C	**-2.769481**	**-3.039248**	**-2.120510**
C	**-1.485707**	**-2.554232**	**-1.794218**
N	**1.566807**	**-1.459767**	**1.031333**
N	**2.884741**	**-1.209709**	**0.829663**
C	**3.624242**	**-2.145086**	**1.486649**
C	**2.769834**	**-3.037763**	**2.122718**
C	**1.486027**	**-2.552487**	**1.796937**
H	**0.505655**	**-0.130137**	**-3.524720**
H	**4.565625**	**0.908153**	**-2.463972**
C	**2.923395**	**0.999772**	**-5.008159**
H	**-4.607026**	**2.326921**	**-1.525145**
C	**-2.822858**	**4.581934**	**-2.547899**
H	**-0.351824**	**3.139648**	**-1.476837**
H	**0.352109**	**3.141349**	**1.473573**
C	**2.822997**	**4.583056**	**2.545684**
H	**4.606975**	**2.326943**	**1.524768**
H	**0.507591**	**-2.939153**	**2.078590**
C	**3.134846**	**-4.231112**	**2.955894**
H	**4.709295**	**-2.114382**	**1.471425**
H	**-0.507226**	**-2.941393**	**-2.075033**
C	**-3.134393**	**-4.233039**	**-2.953097**
H	**-4.709020**	**-2.114774**	**-1.471015**
H	**-0.505831**	**-0.125790**	**3.525067**
C	**-2.924882**	**1.002319**	**5.007822**
H	**-4.566719**	**0.908085**	**2.463555**
H	**-5.211969**	**-1.471891**	**1.577312**
C	**-8.164926**	**-1.645615**	**0.909873**
H	**-7.794222**	**0.320427**	**-1.390116**
H	**7.794357**	**0.320777**	**1.389643**
C	**8.164998**	**-1.645566**	**-0.910082**
H	**5.211964**	**-1.472048**	**-1.577366**
H	**-4.225784**	**-4.316178**	**-3.066179**
H	**-2.700547**	**-4.173888**	**-3.965265**
H	**-2.776075**	**-5.173570**	**-2.501353**
H	**-2.275866**	**4.611806**	**-3.505320**
H	**-3.891675**	**4.713033**	**-2.774190**
H	**-2.498806**	**5.459045**	**-1.962315**
H	**-3.908918**	**1.487345**	**5.093871**
H	**-2.914439**	**0.149889**	**5.708301**
H	**-2.168113**	**1.721496**	**5.361900**
H	**4.226322**	**-4.315156**	**3.067468**
H	**2.702540**	**-4.170616**	**3.968646**
H	**2.774993**	**-5.171724**	**2.505549**
H	**2.164191**	**1.715772**	**-5.363426**
H	**3.905682**	**1.488375**	**-5.093986**
H	**2.916643**	**0.146651**	**-5.707855**
H	**2.500079**	**5.460113**	**1.959389**
H	**2.275040**	**4.613673**	**3.502527**
H	**3.891661**	**4.713608**	**2.773008**
H	**8.665675**	**-2.258939**	**-0.142215**
H	**7.851755**	**-2.321051**	**-1.720605**
H	**8.927388**	**-0.963811**	**-1.324312**
H	**-7.851806**	**-2.320386**	**1.721038**
H	**-8.927749**	**-0.963827**	**1.323242**
H	**-8.665037**	**-2.259747**	**0.142240**

Model 11

89

Cd	**-0.000031**	**0.000315**	**-0.000305**
C	**2.779863**	**-2.535009**	**2.692698**
C	**1.480839**	**-2.155989**	**2.301357**
N	**1.558770**	**-1.235285**	**1.327727**
N	**2.883340**	**-1.010601**	**1.082209**
C	**3.645979**	**-1.789243**	**1.898909**
N	**-1.558546**	**1.237284**	**-1.326298**
N	**-2.883072**	**1.011776**	**-1.081312**
C	**-3.645850**	**1.788746**	**-1.899488**
C	**-2.779842**	**2.533959**	**-2.693972**
C	**-1.480781**	**2.156325**	**-2.301460**
B	**3.361059**	**0.003904**	**0.002180**
N	**2.880105**	**1.445674**	**0.338728**
N	**1.555029**	**1.769049**	**0.408806**
C	**1.475146**	**3.073468**	**0.714756**
C	**2.773292**	**3.604523**	**0.845204**
C	**3.641008**	**2.544545**	**0.600108**
B	**-3.361088**	**-0.003349**	**-0.002162**
N	**-2.884161**	**0.425404**	**1.416455**
N	**-1.559893**	**0.528768**	**1.733876**
C	**-1.483102**	**0.916991**	**3.016463**
C	**-2.782565**	**1.068594**	**3.538756**
C	**-3.647772**	**0.748594**	**2.496829**
N	**1.559533**	**-0.529464**	**-1.733583**
N	**2.883833**	**-0.426294**	**-1.415968**
C	**3.647513**	**-0.749753**	**-2.496137**
C	**2.782429**	**-1.069610**	**-3.538207**
C	**1.482898**	**-0.917786**	**-3.016167**
N	**-1.554996**	**-1.768287**	**-0.409416**
N	**-2.880166**	**-1.444993**	**-0.339991**
C	**-3.640929**	**-2.544286**	**-0.599694**
C	**-2.773070**	**-3.604414**	**-0.843710**
C	**-1.474960**	**-3.073038**	**-0.714097**
H	**4.563444**	**0.005652**	**0.002786**
H	**-4.563449**	**-0.005295**	**-0.003215**
C	**-0.172086**	**2.655000**	**-2.839718**
C	**-5.143629**	**1.798797**	**-1.901570**
H	**-3.055354**	**3.256053**	**-3.458335**
C	**5.145373**	**-0.745446**	**-2.504036**
H	**3.058825**	**-1.373184**	**-4.544688**
C	**0.174941**	**-1.136149**	**-3.718012**
C	**-0.164966**	**-3.786333**	**-0.875482**
H	**-3.046762**	**-4.628532**	**-1.084156**
C	**-5.138769**	**-2.552352**	**-0.609565**
C	**-0.175016**	**1.136558**	**3.717714**
H	**-3.058834**	**1.372232**	**4.545246**
C	**-5.145617**	**0.742612**	**2.505462**
C	**0.165245**	**3.787041**	**0.875686**
H	**3.047090**	**4.628390**	**1.086680**
C	**5.138819**	**2.553149**	**0.608963**
C	**0.172188**	**-2.655126**	**2.839341**
H	**3.055271**	**-3.258517**	**3.455730**
C	**5.143822**	**-1.799517**	**1.900596**
H	**0.338646**	**4.843060**	**1.128710**
H	**-0.437200**	**3.748865**	**-0.044511**
H	**-0.449717**	**3.339511**	**1.671046**
H	**-0.351293**	**1.442440**	**4.759158**
H	**0.442289**	**0.225587**	**3.726658**
H	**0.426273**	**1.917399**	**3.227897**
H	**0.347351**	**-3.410252**	**3.619309**
H	**-0.426810**	**-1.842465**	**3.277463**
H	**-0.447075**	**-3.111109**	**2.052220**
H	**0.351485**	**-1.458797**	**-4.754338**
H	**-0.434498**	**-1.903998**	**-3.217989**
H	**-0.434395**	**-0.220020**	**-3.742951**
H	**-0.338331**	**-4.842104**	**-1.129521**
H	**0.449720**	**-3.337777**	**-1.670502**
H	**0.437634**	**-3.749156**	**0.044649**
H	**-0.347202**	**3.408298**	**-3.621449**
H	**0.446110**	**3.113046**	**-2.052950**
H	**0.427968**	**1.841863**	**-3.275540**
H	**-5.503270**	**2.513145**	**-2.655994**
H	**-5.564386**	**0.809917**	**-2.143224**
H	**-5.557746**	**2.099092**	**-0.926054**
H	**-5.506826**	**1.043236**	**3.499423**
H	**-5.567329**	**1.441375**	**1.765754**
H	**-5.557052**	**-0.254525**	**2.282465**
H	**5.503564**	**-2.513376**	**2.655434**
H	**5.557773**	**-2.100459**	**0.925200**
H	**5.564384**	**-0.810412**	**2.141521**
H	**5.506767**	**-1.046011**	**-3.497940**
H	**5.558089**	**0.250950**	**-2.280131**
H	**5.565602**	**-1.445252**	**-1.764463**
H	**-5.497497**	**-3.563425**	**-0.850019**
H	**-5.561351**	**-2.265803**	**0.366465**
H	**-5.551731**	**-1.858838**	**-1.359063**
H	**5.497192**	**3.564631**	**0.848223**
H	**5.552691**	**1.860579**	**1.358869**
H	**5.560740**	**2.265799**	**-0.367094**

Model 12

53

Cd	**0.000061**	**0.000513**	**-0.004981**
N	**-1.566412**	**0.773044**	**1.615461**
N	**-1.562727**	**-1.788764**	**-0.140788**
N	**1.574240**	**-0.997745**	**-1.489919**
N	**-1.574566**	**1.015110**	**-1.478425**
N	**1.566392**	**-0.790328**	**1.606779**
N	**1.563029**	**1.790686**	**-0.120699**
N	**-2.882273**	**-1.471494**	**-0.109533**
N	**-2.885474**	**0.631083**	**1.328695**
N	**-2.891982**	**0.826385**	**-1.211060**
B	**-3.385008**	**-0.006378**	**0.003816**
H	**-4.595450**	**-0.010936**	**0.006323**
N	**2.885457**	**-0.646488**	**1.320951**
N	**2.891739**	**-0.812009**	**-1.220912**
N	**2.882511**	**1.472831**	**-0.092438**
B	**3.385003**	**0.006467**	**0.003614**
H	**4.595447**	**0.010611**	**0.006045**
C	**1.485598**	**3.124348**	**-0.209703**
C	**3.628377**	**2.601646**	**-0.163110**
C	**2.771697**	**3.693173**	**-0.239975**
H	**0.511398**	**3.607942**	**-0.248269**
H	**4.713567**	**2.546303**	**-0.154066**
H	**3.039546**	**4.743307**	**-0.307962**
C	**-1.489860**	**1.352728**	**2.819780**
C	**-3.632353**	**1.119049**	**2.348439**
C	**-2.776403**	**1.595744**	**3.334024**
H	**-4.717548**	**1.091531**	**2.299117**
H	**-3.045029**	**2.051229**	**4.282459**
H	**-0.515617**	**1.565446**	**3.255656**
C	**1.489858**	**-1.385275**	**2.803648**
C	**3.632345**	**-1.148237**	**2.333968**
C	**2.776411**	**-1.636333**	**3.313975**
H	**0.515624**	**-1.602226**	**3.237448**
H	**3.045074**	**-2.104075**	**4.256415**
H	**4.717549**	**-1.121474**	**2.284366**
C	**1.504754**	**-1.741170**	**-2.601101**
C	**3.644388**	**-1.436940**	**-2.158230**
C	**2.794246**	**-2.050684**	**-3.070287**
H	**0.533133**	**-2.016729**	**-3.006606**
H	**3.068327**	**-2.634458**	**-3.943940**
H	**4.729224**	**-1.400043**	**-2.107935**
C	**-1.505478**	**1.770569**	**-2.581496**
C	**-3.644949**	**1.461469**	**-2.141285**
C	**-2.795119**	**2.085094**	**-3.046896**
H	**-0.534015**	**2.050702**	**-2.984239**
H	**-3.069500**	**2.678424**	**-3.913991**
H	**-4.729768**	**1.424055**	**-2.091021**
C	**-1.484992**	**-3.121252**	**-0.245567**
C	**-3.627893**	**-2.599508**	**-0.193990**
C	**-2.770973**	**-3.689910**	**-0.283330**
H	**-0.510666**	**-3.604162**	**-0.289186**
H	**-3.038576**	**-4.739227**	**-0.363791**
H	**-4.713104**	**-2.544518**	**-0.184883**

Model 13

67

Cd	**-0.000889**	**0.010044**	**-0.078723**
C	**2.585808**	**3.706648**	**0.123644**
C	**1.402725**	**3.087467**	**-0.315582**
N	**1.579192**	**1.767379**	**-0.448260**
N	**2.870131**	**1.505538**	**-0.107939**
C	**3.488512**	**2.661310**	**0.255853**
N	**-1.558737**	**-1.806740**	**-0.052345**
N	**-2.848454**	**-1.489434**	**0.241085**
C	**-3.442523**	**-2.535782**	**0.875526**
C	**-2.524931**	**-3.572069**	**0.973263**
C	**-1.358734**	**-3.057389**	**0.380443**
B	**3.420027**	**0.041701**	**0.028608**
N	**2.903115**	**-0.873407**	**-1.139591**
N	**1.586881**	**-1.119793**	**-1.370220**
C	**1.519943**	**-2.004338**	**-2.370176**
C	**2.810245**	**-2.356136**	**-2.803505**
C	**3.658687**	**-1.617847**	**-1.991193**
B	**-3.420739**	**-0.042303**	**0.041249**
N	**-2.912186**	**0.592257**	**-1.303690**
N	**-1.599626**	**0.816928**	**-1.574926**
C	**-1.541846**	**1.447038**	**-2.752477**
C	**-2.834542**	**1.651548**	**-3.265397**
C	**-3.674652**	**1.097313**	**-2.310414**
N	**1.567230**	**-0.516881**	**1.629239**
N	**2.911068**	**-0.524694**	**1.393333**
C	**3.563149**	**-1.010782**	**2.481875**
C	**2.620505**	**-1.330246**	**3.450101**
C	**1.387054**	**-1.004217**	**2.861827**
N	**-1.582197**	**0.886741**	**1.475734**
N	**-2.924712**	**0.828294**	**1.239923**
C	**-3.586635**	**1.552846**	**2.179467**
C	**-2.651780**	**2.099143**	**3.048867**
C	**-1.412782**	**1.652681**	**2.559353**
N	**4.951338**	**0.100308**	**-0.085247**
N	**-4.950182**	**-0.150663**	**-0.056384**
H	**-0.383054**	**-3.521508**	**0.249076**
H	**-4.473484**	**-2.475479**	**1.209134**
H	**-2.682551**	**-4.554355**	**1.408478**
H	**4.642760**	**-1.106415**	**2.458731**
H	**2.805590**	**-1.743087**	**4.437239**
H	**0.378654**	**-1.094256**	**3.261294**
H	**-0.407621**	**1.843018**	**2.930730**
H	**-2.845237**	**2.731861**	**3.909898**
H	**-4.666789**	**1.630982**	**2.129228**
H	**-0.574179**	**1.719669**	**-3.169445**
H	**-3.120816**	**2.135273**	**-4.194341**
H	**-4.757677**	**1.039220**	**-2.277495**
H	**0.548057**	**-2.340931**	**-2.726150**
H	**3.089453**	**-3.048642**	**-3.591789**
H	**4.742545**	**-1.580835**	**-1.958010**
H	**0.431397**	**3.525323**	**-0.538308**
H	**2.763484**	**4.760448**	**0.316112**
H	**4.524441**	**2.664239**	**0.579097**
N	**5.765411**	**-0.772688**	**0.570881**
C	**6.983125**	**-0.587724**	**0.066470**
C	**6.983150**	**0.397767**	**-0.948594**
C	**5.664380**	**0.805181**	**-1.020152**
H	**5.183378**	**1.529506**	**-1.670918**
H	**7.819099**	**0.762641**	**-1.538655**
H	**7.818242**	**-1.169261**	**0.454567**
C	**-5.647900**	**-1.068317**	**-0.798211**
C	**-6.972865**	**-0.675946**	**-0.827221**
C	**-6.992394**	**0.522300**	**-0.075188**
N	**-5.780097**	**0.840673**	**0.372502**
H	**-7.838060**	**1.166145**	**0.162675**
H	**-7.800529**	**-1.183456**	**-1.314606**
H	**-5.152282**	**-1.918608**	**-1.257276**

Model 14

39

Cd	**-0.007735**	**-0.917485**	**0.040310**
C	**-2.888044**	**-0.912998**	**0.912895**
S	**-2.348960**	**-1.997699**	**-0.355439**
S	**2.322672**	**-2.012235**	**0.459539**
C	**2.871984**	**-0.961675**	**-0.832948**
N	**4.162881**	**-0.988533**	**-1.232913**
N	**-4.179533**	**-0.917523**	**1.311919**
S	**-1.732741**	**0.173767**	**1.662206**
S	**1.727724**	**0.120899**	**-1.604920**
C	**4.690986**	**-0.160041**	**-2.346854**
C	**5.924854**	**0.651746**	**-1.902338**
H	**4.964142**	**-0.843209**	**-3.167096**
H	**3.893184**	**0.493412**	**-2.700501**
C	**7.014415**	**-0.258005**	**-1.296816**
H	**6.312717**	**1.196893**	**-2.773702**
H	**5.608789**	**1.402170**	**-1.163813**
C	**6.422434**	**-1.138740**	**-0.176443**
H	**7.431740**	**-0.903091**	**-2.086120**
H	**7.845006**	**0.346286**	**-0.909348**
C	**5.177325**	**-1.909959**	**-0.659820**
H	**7.164058**	**-1.867048**	**0.179169**
H	**6.141693**	**-0.514465**	**0.683737**
H	**5.459168**	**-2.624666**	**-1.449685**
H	**4.716296**	**-2.468632**	**0.154945**
C	**-4.700064**	**-0.059466**	**2.406957**
C	**-5.925810**	**0.754253**	**1.943836**
H	**-4.980134**	**-0.721604**	**3.241997**
H	**-3.896081**	**0.593871**	**2.746517**
C	**-7.023851**	**-0.158211**	**1.358006**
H	**-6.308735**	**1.322657**	**2.802495**
H	**-5.602192**	**1.484921**	**1.188954**
C	**-6.439984**	**-1.068911**	**0.257527**
H	**-7.447486**	**-0.781805**	**2.161106**
H	**-7.848557**	**0.445254**	**0.956947**
C	**-5.202570**	**-1.841366**	**0.758345**
H	**-7.188415**	**-1.797684**	**-0.082531**
H	**-6.152909**	**-0.466315**	**-0.615924**
H	**-5.491589**	**-2.536109**	**1.563290**
H	**-4.746622**	**-2.421951**	**-0.043866**

(For models 15 and 16 contributions of several configurational isomers has been teaken into account. The corresponding averaged weights are also given together the relevant coordinates.)

Model 15A avgd weight 37%

45

Cd	**-0.0076**	**-0.8342**	**0.0376**
C	**5.1839**	**-1.6956**	**-0.3682**
C	**4.7441**	**0.0547**	**-2.0989**
C	**5.9583**	**0.8416**	**-1.5694**
C	**7.0171**	**-0.0434**	**-0.9035**
C	**6.3666**	**-0.8989**	**0.1874**
C	**2.8888**	**-0.8311**	**-0.7020**
C	**-2.9036**	**-0.7854**	**0.7766**
C	**-5.2073**	**-1.6342**	**0.4621**
C	**-6.3821**	**-0.8383**	**-0.1112**
C	**-7.0238**	**0.0480**	**0.9602**
C	**-5.9561**	**0.9370**	**1.6061**
C	**-4.7497**	**0.1501**	**2.1532**
C	**5.0226**	**-0.7605**	**-3.3685**
C	**-5.0362**	**-0.6336**	**3.4407**
N	**4.1974**	**-0.8111**	**-1.0179**
N	**-4.2120**	**-0.7452**	**1.0919**
S	**2.2939**	**-1.8875**	**0.5617**
S	**-2.3195**	**-1.8758**	**-0.4631**
S	**-1.7600**	**0.2517**	**1.6036**
S	**1.7556**	**0.1986**	**-1.5522**
H	**4.6733**	**-2.2533**	**0.4231**
H	**-4.7025**	**-2.2145**	**-0.3165**
H	**3.9524**	**0.7759**	**-2.3334**
H	**6.3916**	**1.4146**	**-2.4057**
H	**5.5924**	**1.5790**	**-0.8338**
H	**7.4968**	**-0.6989**	**-1.6525**
H	**7.8192**	**0.5823**	**-0.4793**
H	**7.0917**	**-1.6052**	**0.6242**
H	**6.0080**	**-0.2532**	**1.0085**
H	**5.5372**	**-2.4277**	**-1.1164**
H	**-3.9508**	**0.8684**	**2.3714**
H	**-6.3834**	**1.5330**	**2.4292**
H	**-5.5829**	**1.6541**	**0.8541**
H	**-7.5099**	**-0.5857**	**1.7237**
H	**-7.8197**	**0.6720**	**0.5219**
H	**-7.1144**	**-1.5469**	**-0.5321**
H	**-6.0172**	**-0.2147**	**-0.9466**
H	**-5.5678**	**-2.3457**	**1.2265**
H	**-5.3584**	**0.0628**	**4.2313**
H	**-5.8282**	**-1.3890**	**3.3195**
H	**-4.1240**	**-1.1423**	**3.7877**
H	**5.3517**	**-0.0853**	**-4.1745**
H	**5.8071**	**-1.5209**	**-3.2303**
H	**4.1054**	**-1.2677**	**-3.7041**

Model 15B avgd weight 31%

45

Cd	**0.0269**	**-0.7813**	**-0.0004**
C	**-4.7363**	**0.4192**	**1.9295**
C	**-5.1698**	**-1.5952**	**0.5108**
C	**-6.3925**	**-0.8719**	**-0.0865**
C	**-7.0050**	**0.1706**	**0.8542**
C	**-5.9252**	**1.1560**	**1.3084**
C	**-2.8762**	**-0.6569**	**0.7032**
C	**2.9304**	**-0.8654**	**-0.7061**
C	**5.2298**	**-1.6432**	**-0.2224**
C	**6.4112**	**-0.7635**	**0.1934**
C	**7.0585**	**-0.0978**	**-1.0240**
C	**5.9969**	**0.6634**	**-1.8249**
C	**4.7862**	**-0.2044**	**-2.2193**
C	**5.0709**	**-1.2149**	**-3.3378**
C	**-5.5123**	**-2.6170**	**1.6029**
N	**-4.1863**	**-0.5932**	**1.0074**
N	**4.2414**	**-0.8831**	**-1.0114**
S	**-1.7567**	**0.5318**	**1.3346**
S	**1.7952**	**-0.0048**	**-1.7248**
S	**2.3347**	**-1.6994**	**0.7138**
S	**-2.2658**	**-1.9349**	**-0.3275**
H	**-3.9314**	**1.1126**	**2.1931**
H	**4.7199**	**-2.0620**	**0.6511**
H	**-4.6663**	**-2.1318**	**-0.3016**
H	**3.9919**	**0.4648**	**-2.5696**
H	**6.4287**	**1.0944**	**-2.7432**
H	**5.6280**	**1.5101**	**-1.2200**
H	**7.5376**	**-0.8677**	**-1.6554**
H	**7.8601**	**0.5904**	**-0.7102**
H	**7.1385**	**-1.3873**	**0.7391**
H	**6.0527**	**0.0072**	**0.8987**
H	**5.5844**	**-2.4904**	**-0.8368**
H	**-5.0503**	**-0.0935**	**2.8566**
H	**-6.3230**	**1.8684**	**2.0500**
H	**-5.5692**	**1.7491**	**0.4475**
H	**-7.4509**	**-0.3226**	**1.7367**
H	**-7.8265**	**0.7015**	**0.3461**
H	**-7.1382**	**-1.6313**	**-0.3741**
H	**-6.0734**	**-0.3715**	**-1.0175**
H	**5.3999**	**-0.6797**	**-4.2428**
H	**5.8579**	**-1.9382**	**-3.0737**
H	**4.1564**	**-1.7740**	**-3.5872**
H	**-6.1843**	**-3.3864**	**1.1902**
H	**-4.5984**	**-3.1182**	**1.9558**
H	**-6.0167**	**-2.1651**	**2.4711**

Model 15C avgd weight 32%

45

Cd	**0.0361**	**-0.6247**	**-0.0733**
C	**-4.6807**	**0.2509**	**2.1319**
C	**-5.1338**	**-1.5624**	**0.4688**
C	**-6.3793**	**-0.7840**	**0.0037**
C	**-6.9807**	**0.1070**	**1.0951**
C	**-5.9019**	**1.0399**	**1.6527**
C	**-2.8465**	**-0.6264**	**0.7195**
C	**2.9182**	**-0.6793**	**-0.8659**
C	**5.1927**	**-1.6411**	**-0.5983**
C	**6.4484**	**-0.8710**	**-0.1469**
C	**7.0615**	**-0.0077**	**-1.2539**
C	**5.9951**	**0.9292**	**-1.8284**
C	**4.7637**	**0.1478**	**-2.2937**
C	**5.4813**	**-2.8198**	**-1.5373**
C	**-5.4376**	**-2.7201**	**1.4288**
N	**-4.1475**	**-0.6203**	**1.0668**
N	**4.2190**	**-0.6969**	**-1.2133**
S	**-1.7138**	**0.4667**	**1.4869**
S	**1.8001**	**0.4149**	**-1.6529**
S	**2.3193**	**-1.7553**	**0.3793**
S	**-2.2622**	**-1.7325**	**-0.5061**
H	**-3.8784**	**0.9210**	**2.4570**
H	**4.7005**	**-2.0380**	**0.2971**
H	**-4.6470**	**-1.9817**	**-0.4193**
H	**5.0270**	**-0.5056**	**-3.1449**
H	**3.9703**	**0.8225**	**-2.6311**
H	**6.3886**	**1.5036**	**-2.6834**
H	**5.6853**	**1.6612**	**-1.0617**
H	**7.4662**	**-0.6470**	**-2.0591**
H	**7.9123**	**0.5696**	**-0.8569**
H	**7.1817**	**-1.5984**	**0.2388**
H	**6.1667**	**-0.2227**	**0.7011**
H	**-4.9523**	**-0.3836**	**2.9947**
H	**-6.2875**	**1.6346**	**2.4972**
H	**-5.5826**	**1.7539**	**0.8730**
H	**-7.3935**	**-0.5124**	**1.9116**
H	**-7.8239**	**0.6883**	**0.6879**
H	**-7.1222**	**-1.5083**	**-0.3689**
H	**-6.0893**	**-0.1547**	**-0.8557**
H	**6.1397**	**-3.5426**	**-1.0297**
H	**4.5460**	**-3.3376**	**-1.7984**
H	**5.9795**	**-2.5130**	**-2.4701**
H	**-6.1056**	**-3.4432**	**0.9342**
H	**-4.5092**	**-3.2454**	**1.6992**
H	**-5.9317**	**-2.3901**	**2.3558**

Model 16A avgd weight 29%

45

Cd	3.6038	-4.2110	1.9450
C	5.9578	-8.6696	3.5395
C	6.4588	-7.0857	5.3411
C	5.8765	-8.0260	6.4108
C	5.9693	-9.4848	5.9357
C	5.3595	-9.6632	4.5404
C	5.1202	-6.3364	3.3900
C	2.0917	-2.0867	0.4940
C	2.0257	-0.2067	-1.1260
C	1.8743	1.2534	-0.6660
C	0.3922	1.5735	-0.4155
C	-0.2541	0.5497	0.5248
C	-0.0292	-0.8822	0.0276
C	2.5103	2.2048	-1.6825
C	6.5744	-7.8072	7.7553
N	5.8122	-7.2920	4.0366
N	1.4071	-1.1369	-0.1689
S	4.3640	-6.6824	1.8506
S	3.8080	-2.2912	0.2219
S	1.2729	-3.1314	1.6343
S	4.9702	-4.7350	4.0794
H	4.2671	-9.5094	4.5807
H	0.1724	0.6431	1.5387
H	2.4169	1.3472	0.2932
H	-1.3383	0.7294	0.6128
H	5.4767	-8.7445	2.5592
H	3.0799	-0.4766	-1.2487
H	7.5397	-7.2875	5.2159
H	6.3420	-6.0358	5.6301
H	4.8076	-7.7642	6.5215
H	7.0347	-9.7856	5.9119
H	5.4725	-10.1512	6.6607
H	5.5276	-10.6875	4.1684
H	7.0384	-8.8641	3.4082
H	-0.5301	-1.0300	-0.9471
H	-0.4262	-1.6218	0.7301
H	-0.1423	1.5702	-1.3851
H	0.2887	2.5917	-0.0044
H	1.5214	-0.3438	-2.1013
H	6.1488	-8.4648	8.5300
H	7.6534	-8.0298	7.6856
H	6.4672	-6.7664	8.1010
H	2.4220	3.2515	-1.3502
H	3.5809	1.9864	-1.8252
H	2.0160	2.1249	-2.6663

Model 16B avgd weight 35%

45

Cd	3.6846	-4.1403	2.0252
C	6.4306	-7.1017	5.4407
C	5.9728	-8.6465	3.5919
C	5.3623	-9.7003	4.5359
C	5.9623	-9.5366	5.9475
C	5.8488	-8.0925	6.4543
C	5.1526	-6.3032	3.4657
C	2.1512	-2.0268	0.5794
C	0.0104	-0.8699	0.0878
C	-0.2734	0.5771	0.5035
C	0.3490	1.5708	-0.4867
C	1.8493	1.2944	-0.7167
C	2.0495	-0.1872	-1.0908
C	3.8275	-9.6613	4.5277
C	2.7269	1.7118	0.4715
N	5.8023	-7.2824	4.1207
N	1.4569	-1.0850	-0.0850
S	4.4375	-6.6116	1.8984
S	3.8672	-2.2254	0.2967
S	1.3469	-3.0671	1.7334
S	5.0152	-4.7076	4.1715
H	5.6782	-10.6829	4.1420
H	2.1724	1.8778	-1.5975
H	-1.3653	0.7210	0.5589
H	0.1202	0.7405	1.5209
H	5.5233	-8.6956	2.5946
H	3.1114	-0.4318	-1.1987
H	7.5159	-7.2766	5.3182
H	6.2874	-6.0649	5.7611
H	6.3853	-7.9756	7.4106
H	4.7953	-7.8284	6.6464
H	7.0301	-9.8210	5.9168
H	5.4736	-10.2309	6.6511
H	7.0588	-8.8248	3.4875
H	-0.4760	-1.0885	-0.8814
H	-0.3673	-1.5843	0.8261
H	-0.1809	1.4893	-1.4534
H	0.2039	2.6061	-0.1360
H	1.5501	-0.3985	-2.0541
H	3.4159	-10.4393	5.1911
H	3.4350	-8.6893	4.8656
H	3.4337	-9.8351	3.5141
H	2.5791	2.7781	0.7082
H	2.5004	1.1313	1.3797
H	3.7941	1.5586	0.2468

Model 16C avgd weight 28%
45

Cd	3.6452	-4.1408	1.9779
C	2.0086	-0.2201	-1.1657
C	-0.0359	-0.8968	0.0036
C	-0.2545	0.5329	0.5096
C	0.3895	1.5611	-0.4279
C	1.8683	1.2368	-0.6925
C	2.0950	-2.0875	0.4663
C	5.2674	-6.1165	3.5170
C	2.5013	2.1955	-1.7038
C	6.2010	-8.4016	3.7906
C	5.6635	-9.3713	4.8584
C	6.3069	-9.0659	6.2209
C	6.1732	-7.5839	6.5893
C	6.6959	-6.6838	5.4659
C	5.8848	-10.8222	4.4238
N	1.3987	-1.1525	-0.2053
N	6.0177	-7.0009	4.1989
S	3.8099	-2.2849	0.1818
S	4.4769	-6.5896	2.0290
S	5.0756	-4.4813	4.1086
S	1.2937	-3.1185	1.6317
H	4.5757	-9.1890	4.9402
H	2.4182	1.3184	0.2635
H	6.7298	-7.3597	7.5143
H	3.0601	-0.4933	-1.3033
H	5.7026	-8.5568	2.8277
H	-0.5432	-1.0389	-0.9685
H	-0.4291	-1.6390	0.7055
H	-1.3379	0.7149	0.6043
H	0.1771	0.6192	1.5219
H	-0.1516	1.5683	-1.3938
H	0.2934	2.5765	-0.0081
H	1.4912	-0.3496	-2.1352
H	7.7783	-6.8523	5.3152
H	6.5442	-5.6238	5.6926
H	7.3794	-9.3381	6.1782
H	5.8546	-9.6993	7.0023
H	7.2849	-8.5705	3.6456
H	2.4205	3.2390	-1.3597
H	3.5700	1.9738	-1.8562
H	1.9999	2.1290	-2.6850
H	5.1152	-7.3328	6.7800
H	5.4878	-11.5224	5.1761
H	5.3843	-11.0375	3.4660
H	6.9594	-11.0415	4.2990

Model 16D avgd weight 1.6 %

45

Cd	3.601459	-4.212041	1.955259
C	2.044965	-0.139253	-1.045586
N	1.423457	-1.089204	-0.107237
C	-0.023461	-0.865451	0.051704
C	-0.298132	0.556335	0.551297
C	0.357648	1.601951	-0.361128
C	1.858317	1.317867	-0.578862
C	2.099190	-2.062837	0.529593
S	1.268816	-3.137743	1.632968
S	4.951196	-4.738239	4.101414
C	5.108425	-6.337580	3.409717
S	4.368070	-6.679756	1.861292
C	2.715697	1.641281	0.652674
S	3.816493	-2.268275	0.262083
N	5.793593	-7.295281	4.060478
C	6.428638	-7.092606	5.371501
C	5.829446	-8.028831	6.435015
C	5.919934	-9.488030	5.960513
C	5.323708	-9.663874	4.559078
C	5.937630	-8.673249	3.564155
H	4.231847	-9.503792	4.587936
H	-1.389045	0.711400	0.593509
H	2.208480	1.952964	-1.412271
H	5.466462	-8.745404	2.578854
H	3.105154	-0.391944	-1.151488
H	7.509131	-7.302350	5.256978
H	6.316080	-6.042027	5.659361
C	6.514470	-7.813896	7.786710
H	4.760860	-7.761323	6.533933
H	6.983940	-9.794232	5.948081
H	5.412349	-10.152077	6.680169
H	5.489996	-10.689329	4.189576
H	7.018519	-8.873370	3.444578
H	-0.492666	-1.017786	-0.938384
H	-0.424335	-1.618841	0.737117
H	0.075929	0.649617	1.584689
H	-0.153411	1.590002	-1.341350
H	0.219346	2.614760	0.052335
H	1.558674	-0.281503	-2.027938
H	2.580092	2.692424	0.955261
H	2.457956	1.006999	1.515426
H	3.784924	1.482962	0.441933
H	6.077193	-8.468723	8.557269
H	7.592803	-8.042737	7.728073
H	6.409933	-6.772439	8.131340

Model 16E avgd weight 1.5 %

45

Cd	3.508549	-4.166998	2.042821
C	-0.055707	-0.806887	0.048958
N	1.372038	-1.104197	-0.147140
C	2.005383	-0.221945	-1.138103
C	1.898666	1.256033	-0.724074
C	0.428623	1.624685	-0.466415
C	-0.237813	0.644254	0.506162
C	2.038947	-2.047314	0.542616
S	1.200126	-3.048107	1.707835
S	4.837447	-4.705999	4.197045
C	5.024165	-6.294595	3.486901
S	4.294955	-6.629266	1.931738
H	-1.316018	0.856394	0.596728
N	5.722942	-7.248137	4.129532
C	5.959498	-8.595648	3.583332
C	5.437288	-9.692646	4.530795
C	6.064169	-9.505871	5.927587
C	5.875742	-8.076770	6.453110
C	6.369403	-7.041524	5.436969
H	5.800782	-10.650699	4.118254
S	3.752045	-2.286782	0.280891
C	3.903458	-9.744463	4.562656
H	0.198552	0.753787	1.514219
H	2.455551	1.365497	0.225180
C	2.547520	2.156274	-1.778247
H	5.489280	-8.661708	2.596612
H	3.050443	-0.524445	-1.262816
H	7.460832	-7.144977	5.288475
H	6.168625	-6.018982	5.772050
H	6.429324	-7.936311	7.396313
H	4.813654	-7.879662	6.675932
H	7.146377	-9.722777	5.864959
H	5.638338	-10.235706	6.636027
H	7.051203	-8.708403	3.450037
H	-0.566466	-0.969071	-0.918242
H	-0.468240	-1.514626	0.774988
H	-0.116395	1.614191	-1.430253
H	0.359433	2.655517	-0.080271
H	1.487194	-0.376279	-2.103678
H	3.555426	-10.547113	5.233046
H	3.464310	-8.797862	4.914924
H	3.494047	-9.938326	3.558912
H	2.491382	3.215083	-1.479237
H	3.609992	1.903640	-1.925309
H	2.039795	2.057980	-2.753496

Model 16F avgd weight 1.6 %

45

Cd	3.599746	-4.190022	2.017766
C	2.070327	-0.226842	-1.128341
N	1.435066	-1.142065	-0.165823
C	-0.003226	-0.883488	0.004336
C	-0.261014	0.553565	0.489031
C	0.406168	1.557912	-0.463922
C	1.886154	1.227167	-0.683514
C	2.109901	-2.080672	0.522584
S	1.275810	-3.106702	1.669179
S	4.936418	-4.738193	4.164399
C	5.122654	-6.322767	3.444904
S	4.389468	-6.651064	1.890717
H	2.453460	1.385436	0.250167
S	3.829641	-2.288821	0.277466
N	5.825046	-7.278944	4.079470
C	6.445837	-7.092895	5.400258
C	5.869488	-8.075418	6.434239
C	6.003218	-9.517971	5.921379
C	5.414332	-9.671882	4.515144
C	6.005896	-8.640606	3.549585
H	4.318738	-9.539828	4.545358
H	5.607221	-10.682441	4.118644
H	2.326513	1.891075	-1.445724
C	-1.762638	0.807634	0.641396
H	0.215121	0.648652	1.482840
H	5.540872	-8.699184	2.560499
H	3.128567	-0.490619	-1.220754
H	7.533281	-7.265332	5.288045
H	6.298779	-6.054416	5.715419
C	6.542184	-7.878528	7.794913
H	4.793259	-7.841356	6.535994
H	7.075848	-9.792249	5.902055
H	5.514373	-10.215558	6.621922
H	7.092112	-8.809604	3.429142
H	-0.491216	-1.039005	-0.976748
H	-0.412534	-1.617930	0.706069
H	-0.123410	1.533843	-1.436071
H	0.294843	2.582850	-0.072165
H	1.588667	-0.389600	-2.110401
H	6.118408	-8.564965	8.545324
H	7.626431	-8.077639	7.736808
H	6.408476	-6.849851	8.166663
H	-1.952658	1.828745	1.008997
H	-2.285978	0.699169	-0.324516
H	-2.221415	0.103030	1.353648

Model 16G avgd weight 1.8 %

45

Cd	**3.708815**	**-4.148309**	**2.008063**
C	**2.098016**	**-0.174357**	**-1.085269**
N	**1.489845**	**-1.084435**	**-0.099161**
C	**0.040305**	**-0.872109**	**0.055377**
C	**-0.276928**	**0.569056**	**0.500684**
C	**0.359694**	**1.565434**	**-0.489006**
C	**1.853818**	**1.287531**	**-0.698299**
C	**2.180106**	**-2.032265**	**0.560941**
S	**1.367813**	**-3.091756**	**1.692440**
S	**5.055867**	**-4.692907**	**4.148904**
C	**5.211944**	**-6.287724**	**3.445622**
S	**4.478874**	**-6.616055**	**1.891296**
H	**2.425443**	**1.515429**	**0.217029**
N	**5.890513**	**-7.251861**	**4.093641**
C	**6.498716**	**-7.068489**	**5.421246**
C	**5.867990**	**-8.031410**	**6.432818**
C	**5.957778**	**-9.484127**	**5.950651**
C	**5.387824**	**-9.645178**	**4.532089**
C	**6.040130**	**-8.623585**	**3.584794**
H	**4.307371**	**-9.411079**	**4.562893**
S	**3.899540**	**-2.219523**	**0.294371**
C	**5.565025**	**-11.066617**	**3.992784**
H	**2.259002**	**1.934461**	**-1.494018**
H	**-1.374537**	**0.674326**	**0.433408**
C	**0.132870**	**0.823797**	**1.957899**
H	**5.603443**	**-8.677850**	**2.581991**
H	**3.166721**	**-0.398961**	**-1.159811**
H	**7.580735**	**-7.273452**	**5.322558**
H	**6.375909**	**-6.024267**	**5.725657**
H	**6.375442**	**-7.910038**	**7.404171**
H	**4.812387**	**-7.744885**	**6.581672**
H	**7.017397**	**-9.805222**	**5.947323**
H	**5.429810**	**-10.154368**	**6.649548**
H	**7.123160**	**-8.833249**	**3.498654**
H	**-0.427934**	**-1.070345**	**-0.926244**
H	**-0.347764**	**-1.605015**	**0.770372**
H	**-0.158582**	**1.482036**	**-1.461837**
H	**0.205676**	**2.599595**	**-0.138809**
H	**1.633701**	**-0.389840**	**-2.066065**
H	**5.082131**	**-11.802133**	**4.655811**
H	**5.121788**	**-11.175593**	**2.989783**
H	**6.633327**	**-11.335005**	**3.919976**
H	**-0.120206**	**1.853414**	**2.259040**
H	**-0.386072**	**0.132557**	**2.640318**
H	**1.214017**	**0.683749**	**2.114726**

Model 16H avgd weight 1.6 %

45

Cd	**3.645202**	**-4.140765**	**1.977900**
C	**2.008574**	**-0.220142**	**-1.165740**
N	**1.398685**	**-1.152548**	**-0.205326**
C	**-0.035863**	**-0.896824**	**0.003589**
C	**-0.254525**	**0.532909**	**0.509624**
C	**0.389501**	**1.561128**	**-0.427888**
C	**1.868262**	**1.236768**	**-0.692526**
C	**2.094996**	**-2.087451**	**0.466330**
S	**3.809870**	**-2.284883**	**0.181762**
S	**4.476855**	**-6.589574**	**2.028981**
C	**5.267374**	**-6.116511**	**3.517014**
S	**5.075567**	**-4.481278**	**4.108565**
C	**2.501303**	**2.195454**	**-1.703771**
N	**6.017708**	**-7.000907**	**4.198869**
C	**6.200967**	**-8.401617**	**3.790596**
C	**5.663532**	**-9.371282**	**4.858408**
C	**6.306945**	**-9.065929**	**6.220900**
C	**6.173159**	**-7.583920**	**6.589316**
C	**6.695874**	**-6.683789**	**5.465935**
S	**1.293728**	**-3.118450**	**1.631678**
H	**4.575744**	**-9.188998**	**4.940179**
H	**2.418245**	**1.318392**	**0.263459**
C	**5.884754**	**-10.822191**	**4.423807**
H	**6.729828**	**-7.359661**	**7.514293**
H	**3.060088**	**-0.493306**	**-1.303262**
H	**5.702619**	**-8.556819**	**2.827730**
H	**-0.543242**	**-1.038897**	**-0.968486**
H	**-0.429096**	**-1.639041**	**0.705488**
H	**-1.337916**	**0.714895**	**0.604281**
H	**0.177137**	**0.619170**	**1.521926**
H	**-0.151628**	**1.568265**	**-1.393848**
H	**0.293381**	**2.576542**	**-0.008113**
H	**1.491178**	**-0.349575**	**-2.135182**
H	**7.778330**	**-6.852293**	**5.315245**
H	**6.544214**	**-5.623795**	**5.692573**
H	**7.379400**	**-9.338133**	**6.178244**
H	**5.854639**	**-9.699297**	**7.002332**
H	**7.284910**	**-8.570493**	**3.645569**
H	**2.420473**	**3.238997**	**-1.359660**
H	**3.569973**	**1.973839**	**-1.856174**
H	**1.999942**	**2.128969**	**-2.684996**
H	**5.115233**	**-7.332801**	**6.780038**
H	**5.487804**	**-11.522395**	**5.176066**
H	**5.384265**	**-11.037519**	**3.465969**
H	**6.959359**	**-11.041508**	**4.299021**

Model 17

63

Cd	**-0.000206**	**-0.000107**	**-0.204540**
C	**1.675939**	**1.630249**	**2.241666**
N	**1.568359**	**1.123039**	**1.000607**
N	**2.806639**	**1.148075**	**0.425024**
C	**3.699405**	**1.672704**	**1.299482**
C	**3.014091**	**1.992088**	**2.472924**
N	**1.537568**	**-1.358621**	**-1.086953**
N	**2.781801**	**-0.816234**	**-1.240474**
C	**3.656978**	**-1.790606**	**-1.583947**
C	**2.953324**	**-2.995741**	**-1.646950**
C	**1.623605**	**-2.680210**	**-1.324691**
C	**5.110151**	**-1.541245**	**-1.842171**
B	**2.970378**	**0.725871**	**-1.075167**
C	**0.425697**	**-3.577144**	**-1.267110**
C	**5.150983**	**1.859525**	**0.985287**
C	**0.489576**	**1.776157**	**3.144249**
H	**2.069111**	**1.267209**	**-1.702566**
H	**4.070653**	**1.045219**	**-1.464998**
H	**3.433119**	**2.439045**	**3.370699**
H	**-0.418389**	**1.367411**	**2.677825**
H	**0.647469**	**1.253419**	**4.101400**
H	**0.301100**	**2.836616**	**3.379866**
H	**5.297896**	**2.546124**	**0.137108**
H	**5.670189**	**2.275149**	**1.860590**
H	**5.636983**	**0.907837**	**0.719071**
H	**3.355111**	**-3.972629**	**-1.902737**
H	**-0.268769**	**-3.269828**	**-0.471303**
H	**-0.135701**	**-3.554365**	**-2.216285**
H	**0.730967**	**-4.617582**	**-1.082475**
H	**5.258693**	**-0.821575**	**-2.661948**
H	**5.619793**	**-1.132570**	**-0.955156**
H	**5.605946**	**-2.483670**	**-2.115121**
N	**-1.535974**	**1.355896**	**-1.089451**
C	**-1.619929**	**2.677007**	**-1.332334**
C	**-2.947976**	**2.992791**	**-1.658569**
C	**-3.654588**	**1.789215**	**-1.588635**
N	**-2.781627**	**0.815607**	**-1.238981**
C	**-5.106667**	**1.540360**	**-1.853494**
H	**-3.346162**	**3.968446**	**-1.924412**
C	**-0.428190**	**3.579613**	**-1.240968**
H	**-0.662991**	**4.566287**	**-1.665079**
H	**-0.111261**	**3.727114**	**-0.195172**
H	**0.433347**	**3.163322**	**-1.785465**
H	**-5.621040**	**1.134316**	**-0.968031**
H	**-5.600291**	**2.482592**	**-2.131028**
H	**-5.251922**	**0.818841**	**-2.672251**
N	**-1.567141**	**-1.133046**	**0.998516**
N	**-2.807812**	**-1.147509**	**0.426545**
C	**-3.702652**	**-1.661671**	**1.304673**
C	**-3.016946**	**-1.985286**	**2.476976**
C	**-1.676205**	**-1.637054**	**2.241264**
C	**-0.487825**	**-1.794690**	**3.139100**
H	**-3.437576**	**-2.427229**	**3.376492**
C	**-5.156805**	**-1.835331**	**0.994903**
B	**-2.970728**	**-0.726971**	**-1.074624**
H	**-2.069549**	**-1.269526**	**-1.700088**
H	**-4.071694**	**-1.045343**	**-1.463629**
H	**-0.637350**	**-1.271954**	**4.097533**
H	**-0.308109**	**-2.857247**	**3.372038**
H	**0.421909**	**-1.393805**	**2.669355**
H	**-5.677385**	**-2.245662**	**1.871881**
H	**-5.634612**	**-0.879260**	**0.729583**
H	**-5.312336**	**-2.520889**	**0.147435**

Model 18

63

Cd	**0.317371**	**0.102460**	**-0.049544**
S	**2.528054**	**-1.405644**	**0.589289**
S	**2.509784**	**1.370998**	**-0.584523**
B	**-2.971215**	**-0.131587**	**0.059704**
N	**-1.081380**	**-1.370819**	**-1.143126**
N	**-2.413986**	**-1.261578**	**-0.857672**
N	**-1.345534**	**1.674693**	**-0.706999**
N	**-2.637628**	**1.264099**	**-0.538326**
N	**-1.074489**	**-0.130551**	**1.777835**
N	**-2.409468**	**-0.249363**	**1.508028**
N	**4.744176**	**-0.000423**	**0.000388**
C	**-0.924455**	**-2.405325**	**-1.980824**
C	**-2.181090**	**-2.983992**	**-2.242508**
C	**-3.101661**	**-2.234740**	**-1.516120**
C	**0.416948**	**-2.787759**	**-2.525731**
C	**-4.585404**	**-2.418761**	**-1.430992**
C	**-1.379866**	**2.906668**	**-1.233267**
C	**-2.719284**	**3.303824**	**-1.409534**
C	**-3.491647**	**2.237409**	**-0.958217**
C	**-0.131719**	**3.671377**	**-1.556475**
C	**-4.984161**	**2.122199**	**-0.915624**
C	**-0.912562**	**-0.240029**	**3.103900**
C	**-2.168345**	**-0.438594**	**3.708954**
C	**-3.093824**	**-0.438279**	**2.669663**
C	**0.432926**	**-0.121550**	**3.750815**
C	**-4.578977**	**-0.612207**	**2.750902**
C	**5.516706**	**1.142699**	**-0.516678**
C	**5.843788**	**2.179212**	**0.558920**
C	**5.545302**	**-1.124102**	**0.517154**
C	**5.892890**	**-2.153459**	**-0.558500**
C	**3.395789**	**-0.020617**	**0.005702**
H	**-4.166722**	**-0.249231**	**0.111543**
H	**-2.395572**	**-3.839690**	**-2.877265**
H	**1.225535**	**-2.476105**	**-1.848313**
H	**0.482468**	**-3.877491**	**-2.666355**
H	**0.594671**	**-2.317104**	**-3.508128**
H	**-4.920009**	**-2.600580**	**-0.397530**
H	**-5.132897**	**-1.537357**	**-1.800669**
H	**-4.882948**	**-3.283405**	**-2.041180**
H	**-3.081625**	**4.246022**	**-1.812423**
H	**0.462782**	**3.166547**	**-2.335160**
H	**-0.384009**	**4.677487**	**-1.921243**
H	**0.516367**	**3.780610**	**-0.672457**
H	**-5.434697**	**3.045366**	**-1.307229**
H	**-5.351260**	**1.280897**	**-1.524739**
H	**-5.358137**	**1.970270**	**0.109322**
H	**-2.378990**	**-0.567908**	**4.767283**
H	**1.234257**	**-0.431657**	**3.063936**
H	**0.633960**	**0.918756**	**4.060058**
H	**0.485710**	**-0.749220**	**4.653385**
H	**-5.119245**	**0.266927**	**2.365643**
H	**-4.924770**	**-1.485487**	**2.175619**
H	**-4.873671**	**-0.758631**	**3.799810**
H	**4.943141**	**1.604506**	**-1.331042**
H	**6.441793**	**0.733412**	**-0.953036**
H	**6.449861**	**2.990921**	**0.124568**
H	**4.920640**	**2.618204**	**0.965661**
H	**6.417389**	**1.736340**	**1.389511**
H	**4.980979**	**-1.598617**	**1.330483**
H	**6.461615**	**-0.692235**	**0.950460**
H	**6.519772**	**-2.949915**	**-0.125427**
H	**4.978158**	**-2.614781**	**-0.959355**
H	**6.452341**	**-1.698886**	**-1.392531**

Model 19

75

Cd	**0.3610**	**0.0371**	**-0.1760**
C	**1.7163**	**-0.4052**	**3.5233**
C	**2.4648**	**-1.4646**	**2.9830**
C	**2.6141**	**-2.6392**	**3.7431**
C	**2.0267**	**-2.7524**	**5.0041**
C	**1.2774**	**-1.6942**	**5.5283**
C	**1.1237**	**-0.5222**	**4.7824**
C	**3.1274**	**-1.3499**	**1.6698**
C	**4.5978**	**-1.4305**	**0.0121**
C	**4.4179**	**-1.8175**	**1.3289**
C	**-2.5089**	**0.4938**	**0.7265**
C	**-4.1187**	**0.3831**	**2.5974**
C	**-4.5558**	**-1.0673**	**2.8150**
C	**0.2448**	**-2.1843**	**-2.7920**
C	**1.0455**	**-2.4490**	**-3.9261**
C	**2.2229**	**-1.7529**	**-3.7023**
C	**-1.0939**	**-2.7232**	**-2.4895**
C	**-2.0092**	**-2.9570**	**-3.5313**
C	**-3.2693**	**-3.4948**	**-3.2658**
C	**-3.6374**	**-3.8090**	**-1.9536**
C	**-2.7344**	**-3.5814**	**-0.9106**
C	**-1.4724**	**-3.0468**	**-1.1750**
C	**3.4063**	**2.2842**	**-2.3964**
C	**2.7272**	**3.4513**	**-2.0873**
C	**1.6770**	**3.0463**	**-1.2320**
C	**0.6748**	**3.9063**	**-0.5755**
C	**0.1962**	**3.6274**	**0.7161**
C	**-0.7326**	**4.4704**	**1.3284**
C	**-1.1952**	**5.6108**	**0.6655**
C	**-0.7229**	**5.9010**	**-0.6183**
C	**0.2029**	**5.0568**	**-1.2329**
C	**-4.8109**	**1.2802**	**0.3497**
C	**-5.5892**	**0.2480**	**-0.4688**
N	**2.5697**	**-0.7298**	**0.6099**
N	**3.4820**	**-0.7822**	**-0.3990**
N	**-3.7548**	**0.7058**	**1.2054**
N	**2.1229**	**-1.1099**	**-2.5163**
N	**0.9137**	**-1.3668**	**-1.9527**
N	**1.7319**	**1.7100**	**-1.0569**
N	**2.7944**	**1.2521**	**-1.7704**
S	**-1.2763**	**-0.1627**	**1.7977**
S	**-2.1067**	**0.8668**	**-0.9124**
B	**3.2097**	**-0.2420**	**-1.8221**
H	**5.4408**	**-1.5590**	**-0.6611**
H	**3.1314**	**-1.6799**	**-4.2937**
H	**4.2879**	**2.1128**	**-3.0076**
H	**-3.2507**	**0.6081**	**3.2330**
H	**4.2248**	**-0.3255**	**-2.4754**
H	**0.8087**	**-3.0967**	**-4.7645**
H	**5.1281**	**-2.3240**	**1.9752**
H	**2.9741**	**4.4622**	**-2.3962**
H	**-4.9286**	**1.0723**	**2.8821**
H	**-4.3316**	**2.0042**	**-0.3237**
H	**-5.4913**	**1.8348**	**1.0146**
H	**-6.3270**	**0.7652**	**-1.1042**
H	**-4.9109**	**-0.3184**	**-1.1237**
H	**-6.1343**	**-0.4606**	**0.1739**
H	**-1.7351**	**-2.6949**	**-4.5555**
H	**-3.9695**	**-3.6641**	**-4.0871**
H	**-4.6232**	**-4.2315**	**-1.7456**
H	**-3.0089**	**-3.8282**	**0.1174**
H	**-0.7691**	**-2.8938**	**-0.3550**
H	**0.5643**	**2.7530**	**1.2545**
H	**-1.0911**	**4.2351**	**2.3329**
H	**-1.9198**	**6.2715**	**1.1470**
H	**-1.0821**	**6.7866**	**-1.1476**
H	**0.5523**	**5.2783**	**-2.2435**
H	**3.1832**	**-3.4752**	**3.3304**
H	**2.1492**	**-3.6743**	**5.5775**
H	**0.8157**	**-1.7831**	**6.5144**
H	**0.5420**	**0.3110**	**5.1825**
H	**1.6138**	**0.5214**	**2.9575**
H	**-4.7844**	**-1.2266**	**3.8818**
H	**-5.4568**	**-1.3170**	**2.2337**
H	**-3.7494**	**-1.7602**	**2.5324**

Model 20

98

Cd	**-0.7200**	**0.2803**	**0.0628**
N	**2.2184**	**1.1698**	**-0.4203**
N	**1.0930**	**1.7943**	**0.0114**
N	**2.0352**	**-0.9289**	**0.9665**
N	**0.8544**	**-0.5957**	**1.5505**
N	**0.2887**	**-0.6514**	**-1.8191**
N	**1.5445**	**-1.0881**	**-1.4999**
N	**3.8887**	**-0.6656**	**-0.7731**
N	**4.8224**	**-0.3848**	**0.1564**
C	**1.3362**	**3.1556**	**-0.0380**
C	**2.6559**	**3.3508**	**-0.5836**
C	**3.1638**	**2.0981**	**-0.7827**
C	**-3.5154**	**-1.2962**	**0.4175**
C	**-4.2801**	**-0.1479**	**0.0916**
C	**-3.7956**	**1.1423**	**-0.1981**
C	**-4.8287**	**2.2644**	**-0.5086**
C	**-5.5838**	**2.6062**	**0.7967**
C	**0.4660**	**4.1159**	**0.4883**
C	**-0.7457**	**3.7189**	**1.2678**
C	**2.7131**	**-1.8319**	**1.7495**
C	**1.9731**	**-2.0920**	**2.8682**
C	**0.7885**	**-1.2750**	**2.7561**
C	**-0.2221**	**-1.0684**	**3.6944**
C	**-1.2618**	**-0.0114**	**3.4896**
C	**1.7451**	**-2.3502**	**-2.0068**
C	**0.6440**	**-2.7304**	**-2.7191**
C	**-0.2859**	**-1.6287**	**-2.6273**
C	**-1.5009**	**-1.4731**	**-3.2908**
C	**-2.2710**	**-0.1917**	**-3.2593**
C	**-4.1144**	**3.5269**	**-1.0199**
C	**-5.8368**	**1.8041**	**-1.5841**
C	**-2.0949**	**-2.5788**	**-4.1084**
C	**-0.2841**	**-1.8568**	**4.9658**
C	**0.7712**	**5.5776**	**0.3815**
C	**-4.2664**	**-2.6278**	**0.7015**
C	**-5.0797**	**-3.0430**	**-0.5443**
C	**-3.2554**	**-3.7381**	**1.0321**
C	**-5.2170**	**-2.4372**	**1.9044**
C	**6.0368**	**-0.3998**	**-0.4879**
C	**5.8181**	**-0.6845**	**-1.8892**
C	**4.4637**	**-0.8305**	**-2.0194**
C	**7.2355**	**-0.1688**	**0.2032**
C	**8.5632**	**-0.2135**	**-0.4804**
C	**7.2325**	**0.1211**	**1.6693**
O	**-2.2512**	**-1.3331**	**0.5079**
O	**-2.5660**	**1.4944**	**-0.2161**
B	**2.4158**	**-0.3791**	**-0.4335**
H	**3.6976**	**-2.1767**	**1.4545**
H	**4.1389**	**1.7901**	**-1.1424**
H	**2.6759**	**-2.8793**	**-1.8259**
H	**2.2576**	**-2.7353**	**3.6943**
H	**3.1735**	**4.2902**	**-0.7462**
H	**0.5264**	**-3.6505**	**-3.2819**
H	**-5.3596**	**-0.2772**	**0.0646**
H	**-6.2981**	**3.4279**	**0.6185**
H	**-6.1478**	**1.7424**	**1.1809**
H	**-4.8844**	**2.9312**	**1.5839**
H	**-4.8613**	**4.2990**	**-1.2668**
H	**-3.4310**	**3.9415**	**-0.2663**
H	**-3.5226**	**3.3175**	**-1.9236**
H	**-6.5271**	**2.6297**	**-1.8253**
H	**-5.3227**	**1.5130**	**-2.5143**
H	**-6.4472**	**0.9505**	**-1.2543**
H	**-5.7160**	**-3.3910**	**2.1454**
H	**-4.6634**	**-2.1110**	**2.8000**
H	**-6.0005**	**-1.6908**	**1.7028**
H	**-5.5896**	**-4.0035**	**-0.3591**
H	**-5.8480**	**-2.3001**	**-0.8068**
H	**-4.4220**	**-3.1744**	**-1.4190**
H	**-3.7906**	**-4.6801**	**1.2361**
H	**-2.5579**	**-3.9067**	**0.1990**
H	**-2.6504**	**-3.4823**	**1.9140**
H	**-3.1391**	**-2.7771**	**-3.7967**
H	**-2.1536**	**-2.3021**	**-5.1803**
H	**-1.5433**	**-3.5256**	**-4.0346**
H	**-2.5884**	**0.0912**	**-4.2811**
H	**-3.2024**	**-0.2931**	**-2.6682**
H	**-1.6938**	**0.6418**	**-2.8396**
H	**-1.8178**	**0.1860**	**4.4191**
H	**-0.8093**	**0.9418**	**3.1523**
H	**-1.9992**	**-0.3018**	**2.7189**
H	**-1.2728**	**-2.3422**	**5.0788**
H	**0.4798**	**-2.6431**	**5.0299**
H	**-0.1720**	**-1.1995**	**5.8508**
H	**-1.2509**	**4.6000**	**1.6922**
H	**-1.4831**	**3.1674**	**0.6591**
H	**-0.4791**	**3.0454**	**2.1089**
H	**-0.0995**	**6.1301**	**-0.0201**
H	**0.9704**	**6.0210**	**1.3783**
H	**1.6324**	**5.7991**	**-0.2630**
H	**3.8575**	**-1.0184**	**-2.8995**
H	**6.5548**	**-0.7644**	**-2.6824**
H	**7.7488**	**1.0775**	**1.8838**
H	**6.2141**	**0.1721**	**2.0730**
H	**7.7965**	**-0.6521**	**2.2288**
H	**9.1083**	**0.7426**	**-0.3517**
H	**9.2172**	**-0.9870**	**-0.0299**
H	**8.4936**	**-0.4201**	**-1.5569**

Model 21

89

Cd	**-0.2821**	**-0.3725**	**0.2053**
C	**0.2377**	**-1.8113**	**-3.0999**
C	**0.5811**	**-3.0310**	**-2.4908**
C	**1.5473**	**-3.8422**	**-3.1128**
C	**2.1547**	**-3.4427**	**-4.3043**
C	**1.8107**	**-2.2233**	**-4.8960**
C	**0.8506**	**-1.4089**	**-4.2875**
C	**-0.0682**	**-3.4803**	**-1.2457**
C	**-1.0161**	**-4.6755**	**0.3671**
C	**-0.3726**	**-4.8040**	**-0.8533**
C	**0.7253**	**2.2697**	**-1.1900**
C	**2.0787**	**1.8894**	**-1.1420**
C	**2.6049**	**0.6543**	**-0.6858**
C	**4.1314**	**0.3771**	**-0.7494**
C	**-0.2837**	**-2.3759**	**4.0795**
C	**0.6126**	**-1.4262**	**4.5429**
C	**0.7100**	**-0.4772**	**3.4996**
C	**1.4928**	**0.7714**	**3.4875**
C	**1.0530**	**1.9083**	**2.7866**
C	**1.7967**	**3.0894**	**2.8093**
C	**2.9857**	**3.1620**	**3.5412**
C	**3.4294**	**2.0394**	**4.2476**
C	**2.6914**	**0.8552**	**4.2193**
C	**0.3298**	**3.6490**	**-1.7853**
C	**-3.8154**	**-0.0264**	**0.5999**
C	**-4.7711**	**-0.6321**	**1.4472**
C	**-4.1100**	**-1.7085**	**2.0138**
C	**-4.0514**	**1.1110**	**-0.3105**
C	**-3.6016**	**1.0827**	**-1.6411**
C	**-3.9175**	**2.1218**	**-2.5184**
C	**-4.6760**	**3.2114**	**-2.0795**
C	**-5.1192**	**3.2549**	**-0.7541**
C	**-4.8134**	**2.2113**	**0.1216**
C	**4.3370**	**-0.8525**	**-1.6614**
C	**4.9649**	**1.5501**	**-1.2907**
C	**4.6056**	**0.0394**	**0.6810**
C	**-0.7255**	**4.2992**	**-0.8666**
C	**1.5096**	**4.6222**	**-1.9531**
C	**-0.2939**	**3.3727**	**-3.1725**
N	**-0.5020**	**-2.6237**	**-0.3005**
N	**-1.0832**	**-3.3604**	**0.6814**
N	**-0.6853**	**-2.0171**	**2.8384**
N	**-0.0812**	**-0.8561**	**2.4754**
N	**-2.6471**	**-0.6959**	**0.6738**
N	**-2.8427**	**-1.7308**	**1.5388**
O	**-0.2788**	**1.5629**	**-0.8166**
O	**1.9206**	**-0.3034**	**-0.2110**
B	**-1.7342**	**-2.7331**	**1.9431**
H	**-0.6768**	**-3.2735**	**4.5487**
H	**-1.4419**	**-5.4231**	**1.0302**
H	**-4.4511**	**-2.4696**	**2.7101**
H	**-2.2294**	**-3.6258**	**2.5923**
H	**1.0962**	**-1.3934**	**5.5142**
H	**-0.1836**	**-5.7182**	**-1.4072**
H	**-5.8105**	**-0.3468**	**1.5766**
H	**0.1112**	**1.8764**	**2.2362**
H	**1.4371**	**3.9617**	**2.2595**
H	**3.5631**	**4.0890**	**3.5624**
H	**4.3593**	**2.0835**	**4.8192**
H	**3.0558**	**-0.0230**	**4.7560**
H	**1.8374**	**-4.7857**	**-2.6458**
H	**2.9065**	**-4.0844**	**-4.7695**
H	**2.2871**	**-1.9102**	**-5.8277**
H	**0.5691**	**-0.4572**	**-4.7434**
H	**-0.5326**	**-1.1803**	**-2.6532**
H	**-5.1595**	**2.2486**	**1.1569**
H	**-5.7076**	**4.1046**	**-0.4002**
H	**-4.9224**	**4.0223**	**-2.7686**
H	**-3.5776**	**2.0757**	**-3.5553**
H	**-3.0272**	**0.2244**	**-1.9926**
H	**2.7950**	**2.6150**	**-1.5060**
H	**5.6751**	**-0.2297**	**0.6715**
H	**4.4740**	**0.8989**	**1.3581**
H	**4.0336**	**-0.8053**	**1.0893**
H	**5.4038**	**-1.1314**	**-1.6877**
H	**3.7573**	**-1.7104**	**-1.2936**
H	**4.0134**	**-0.6421**	**-2.6939**
H	**6.0312**	**1.2705**	**-1.2982**
H	**4.6872**	**1.8130**	**-2.3236**
H	**4.8646**	**2.4513**	**-0.6656**
H	**1.1349**	**5.5927**	**-2.3178**
H	**2.0314**	**4.8014**	**-0.9997**
H	**2.2484**	**4.2632**	**-2.6863**
H	**-0.6452**	**4.3131**	**-3.6298**
H	**0.4446**	**2.9179**	**-3.8535**
H	**-1.1502**	**2.6904**	**-3.0802**
H	**-1.0823**	**5.2442**	**-1.3082**
H	**-1.5849**	**3.6327**	**-0.7187**
H	**-0.2963**	**4.5321**	**0.1228**

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85

Cd	**-0.0077**	**-0.7681**	**0.1834**
C	**-3.6850**	**2.4049**	**-0.6002**
C	**-2.4427**	**3.0104**	**-0.3401**
C	**-2.4081**	**4.3970**	**-0.1025**
C	**-3.5799**	**5.1559**	**-0.1357**
C	**-4.8065**	**4.5443**	**-0.4125**
C	**-4.8535**	**3.1659**	**-0.6446**
C	**-1.2168**	**2.1361**	**-0.2960**
C	**0.0539**	**2.7305**	**-0.4423**
C	**1.3073**	**2.0831**	**-0.3361**
C	**-2.7545**	**-2.6459**	**-0.9496**
C	**-3.3044**	**-3.9015**	**-0.6032**
C	**-2.3576**	**-4.4900**	**0.2185**
C	**-3.3237**	**-1.6519**	**-1.8783**
C	**-2.5060**	**-0.9212**	**-2.7576**
C	**-3.0632**	**-0.0245**	**-3.6702**
C	**-4.4489**	**0.1550**	**-3.7258**
C	**-5.2731**	**-0.5673**	**-2.8573**
C	**-4.7158**	**-1.4616**	**-1.9408**
C	**0.1895**	**-3.3422**	**3.7040**
C	**0.2292**	**-2.2098**	**4.5014**
C	**0.0821**	**-1.1270**	**3.6057**
C	**0.0277**	**0.3085**	**3.9395**
C	**-0.8121**	**1.1953**	**3.2435**
C	**-0.8621**	**2.5461**	**3.5952**
C	**-0.0846**	**3.0309**	**4.6508**
C	**0.7493**	**2.1554**	**5.3535**
C	**0.8059**	**0.8065**	**5.0008**
C	**2.2102**	**-4.5633**	**0.0272**
C	**3.1342**	**-3.9801**	**-0.8239**
C	**2.6288**	**-2.6841**	**-1.0772**
C	**3.2010**	**-1.6632**	**-1.9743**
C	**4.5963**	**-1.5259**	**-2.0828**
C	**5.1550**	**-0.5900**	**-2.9549**
C	**4.3294**	**0.2247**	**-3.7354**
C	**2.9410**	**0.0937**	**-3.6387**
C	**2.3822**	**-0.8432**	**-2.7688**
C	**2.5647**	**2.8961**	**-0.4985**
C	**2.5963**	**4.1484**	**-1.1380**
C	**3.7945**	**4.8536**	**-1.2667**
C	**4.9817**	**4.3235**	**-0.7522**
C	**4.9638**	**3.0757**	**-0.1207**
C	**3.7690**	**2.3656**	**-0.0035**
O	**1.4905**	**0.8468**	**-0.0820**
O	**-1.4503**	**0.8887**	**-0.1299**
N	**-1.5553**	**-2.4964**	**-0.3516**
N	**-1.3182**	**-3.6339**	**0.3568**
N	**0.0348**	**-2.9564**	**2.4171**
N	**-0.0304**	**-1.6001**	**2.3466**
N	**1.4758**	**-2.5101**	**-0.4003**
N	**1.2242**	**-3.6677**	**0.2687**
B	**-0.0212**	**-3.8790**	**1.1688**
H	**0.2505**	**-4.3964**	**3.9592**
H	**2.1749**	**-5.5549**	**0.4696**
H	**-2.3399**	**-5.4620**	**0.7034**
H	**-0.0200**	**-5.0245**	**1.5576**
H	**0.3097**	**-2.1638**	**5.5829**
H	**4.0257**	**-4.4342**	**-1.2451**
H	**-4.2389**	**-4.3315**	**-0.9499**
H	**-1.4422**	**0.8275**	**2.4327**
H	**-1.5211**	**3.2192**	**3.0429**
H	**-0.1278**	**4.0873**	**4.9254**
H	**1.3649**	**2.5259**	**6.1765**
H	**1.4743**	**0.1315**	**5.5397**
H	**5.2461**	**-2.1474**	**-1.4629**
H	**6.2411**	**-0.4921**	**-3.0204**
H	**4.7661**	**0.9596**	**-4.4151**
H	**2.2881**	**0.7220**	**-4.2486**
H	**1.2983**	**-0.9587**	**-2.7192**
H	**-5.3637**	**-2.0123**	**-1.2555**
H	**-6.3567**	**-0.4322**	**-2.8909**
H	**-4.8839**	**0.8552**	**-4.4422**
H	**-2.4119**	**0.5323**	**-4.3474**
H	**-1.4267**	**-1.0797**	**-2.7402**
H	**0.0720**	**3.8004**	**-0.6235**
H	**-1.4645**	**4.8897**	**0.1365**
H	**-3.5348**	**6.2296**	**0.0614**
H	**-5.7223**	**5.1397**	**-0.4412**
H	**-5.8075**	**2.6788**	**-0.8600**
H	**-3.7123**	**1.3295**	**-0.7721**
H	**1.6858**	**4.5711**	**-1.5649**
H	**3.8012**	**5.8208**	**-1.7748**
H	**5.9178**	**4.8789**	**-0.8485**
H	**5.8880**	**2.6518**	**0.2794**
H	**3.7434**	**1.3860**	**0.4731**

Model 23

71

Cd	**-0.4194**	**-0.2006**	**0.2907**
C	**2.2374**	**1.7783**	**2.0765**
C	**2.3840**	**0.6003**	**2.8303**
C	**3.6796**	**0.1642**	**3.1578**
C	**4.7983**	**0.8865**	**2.7383**
C	**4.6418**	**2.0541**	**1.9844**
C	**3.3575**	**2.4966**	**1.6531**
C	**1.2025**	**-0.1531**	**3.2899**
C	**-0.3044**	**-1.2809**	**4.4680**
C	**0.9861**	**-0.7772**	**4.5381**
C	**1.5232**	**1.5865**	**-1.5094**
C	**-1.8630**	**-3.2468**	**-0.4041**
C	**-2.7476**	**-4.1050**	**0.2843**
C	**-2.9169**	**-3.5228**	**1.5301**
C	**-1.3573**	**-3.4105**	**-1.7823**
C	**0.0023**	**-3.2397**	**-2.0930**
C	**0.4564**	**-3.4217**	**-3.4019**
C	**-0.4356**	**-3.7847**	**-4.4148**
C	**-1.7891**	**-3.9674**	**-4.1122**
C	**-2.2471**	**-3.7829**	**-2.8066**
C	**2.5437**	**-0.5953**	**-1.0089**
C	**-4.1218**	**0.4405**	**2.5871**
C	**-4.4885**	**1.4906**	**1.7651**
C	**-3.4378**	**1.6069**	**0.8265**
C	**-3.3694**	**2.5847**	**-0.2782**
C	**-4.5538**	**2.9293**	**-0.9581**
C	**-4.5382**	**3.8732**	**-1.9853**
C	**-3.3377**	**4.4883**	**-2.3552**
C	**-2.1566**	**4.1523**	**-1.6888**
C	**-2.1717**	**3.2134**	**-0.6546**
C	**2.5840**	**0.6818**	**-1.6013**
C	**3.7801**	**-1.5076**	**-1.1714**
C	**1.7177**	**2.9912**	**-2.1166**
N	**0.1014**	**-0.2934**	**2.5254**
N	**-0.8168**	**-0.9822**	**3.2519**
N	**-2.1822**	**-2.3883**	**1.5803**
N	**-1.5315**	**-2.2109**	**0.3961**
N	**-2.4965**	**0.6718**	**1.0824**
N	**-2.9285**	**-0.0393**	**2.1661**
O	**0.3873**	**1.4443**	**-0.9701**
O	**1.6170**	**-1.1184**	**-0.3458**
B	**-2.2281**	**-1.3145**	**2.7070**
H	**-3.5057**	**-3.8345**	**2.3881**
H	**-4.6213**	**-0.0020**	**3.4443**
H	**-0.9001**	**-1.8173**	**5.2012**
H	**-2.8891**	**-1.7612**	**3.6154**
H	**-3.1681**	**-5.0382**	**-0.0769**
H	**-5.3720**	**2.1163**	**1.8417**
H	**1.6646**	**-0.8108**	**5.3848**
H	**0.7103**	**-2.9798**	**-1.3070**
H	**1.5179**	**-3.2874**	**-3.6199**
H	**-0.0779**	**-3.9285**	**-5.4369**
H	**-2.4935**	**-4.2496**	**-4.8981**
H	**-3.3073**	**-3.9109**	**-2.5770**
H	**-5.4903**	**2.4368**	**-0.6882**
H	**-5.4664**	**4.1235**	**-2.5043**
H	**-3.3234**	**5.2249**	**-3.1618**
H	**-1.2120**	**4.6190**	**-1.9724**
H	**-1.2428**	**2.9731**	**-0.1416**
H	**3.8082**	**-0.7592**	**3.7263**
H	**5.7986**	**0.5301**	**2.9942**
H	**5.5183**	**2.6164**	**1.6551**
H	**3.2206**	**3.4047**	**1.0621**
H	**1.2375**	**2.1459**	**1.8404**
H	**3.4850**	**0.9874**	**-2.1233**
F	**4.2828**	**-1.8432**	**0.0282**
F	**3.4293**	**-2.6525**	**-1.8023**
F	**4.7707**	**-0.9408**	**-1.8899**
F	**2.9285**	**3.1717**	**-2.6780**
F	**0.7886**	**3.2414**	**-3.0580**
F	**1.5751**	**3.9294**	**-1.1494**

Model 24

70

Cd	**-0.0724**	**-0.0001**	**0.5013**
C	**1.5864**	**-2.2153**	**-2.8478**
C	**1.7558**	**-2.7249**	**-0.6884**
C	**2.1152**	**-3.1605**	**-1.9826**
C	**1.7552**	**2.7254**	**-0.6877**
C	**2.1139**	**3.1619**	**-1.9818**
C	**1.5855**	**2.2168**	**-2.8473**
C	**-0.6261**	**-0.0005**	**3.1144**
C	**-0.9860**	**-0.0007**	**4.5830**
C	**2.0720**	**3.4002**	**0.6424**
C	**0.7783**	**3.9861**	**1.2541**
C	**2.0724**	**-3.4002**	**0.6415**
C	**3.0726**	**-4.5492**	**0.4048**
C	**-2.2801**	**0.0009**	**-3.2158**
C	**-3.4755**	**0.0007**	**-2.5118**
C	**-3.1060**	**0.0002**	**-1.1499**
C	**-4.0163**	**-0.0005**	**0.0724**
C	**-3.7637**	**-1.2673**	**0.9202**
C	**2.7079**	**-2.3923**	**1.6230**
C	**0.7786**	**-3.9859**	**1.2531**
C	**2.7071**	**2.3918**	**1.6237**
C	**3.0726**	**4.5488**	**0.4062**
C	**-3.7641**	**1.2656**	**0.9215**
C	**-5.4882**	**-0.0005**	**-0.3842**
N	**0.9511**	**-1.2745**	**-2.1173**
N	**1.0492**	**-1.5794**	**-0.7903**
N	**0.9508**	**1.2753**	**-2.1171**
N	**1.0492**	**1.5795**	**-0.7900**
N	**-1.7596**	**-0.0001**	**-1.0612**
N	**-1.2614**	**0.0003**	**-2.3305**
B	**0.2560**	**0.0004**	**-2.6641**
O	**-0.4921**	**1.1060**	**2.5031**
O	**-0.4915**	**-1.1067**	**2.5027**
H	**1.6211**	**-2.1420**	**-3.9311**
H	**1.6200**	**2.1441**	**-3.9307**
H	**-2.0823**	**0.0012**	**-4.2840**
H	**0.3674**	**0.0005**	**-3.8683**
H	**2.6860**	**-4.0417**	**-2.2531**
H	**2.6841**	**4.0436**	**-2.2520**
H	**-4.4762**	**0.0011**	**-2.9292**
H	**-4.4613**	**-1.2944**	**1.7742**
H	**-3.9245**	**-2.1791**	**0.3226**
H	**-2.7420**	**-1.3035**	**1.3262**
H	**-4.4609**	**1.2909**	**1.7762**
H	**-2.7421**	**1.3021**	**1.3267**
H	**-3.9263**	**2.1779**	**0.3252**
H	**-6.1512**	**-0.0005**	**0.4951**
H	**-5.7278**	**0.8920**	**-0.9838**
H	**-5.7278**	**-0.8930**	**-0.9838**
H	**3.3252**	**5.0249**	**1.3666**
H	**4.0087**	**4.1867**	**-0.0482**
H	**2.6512**	**5.3279**	**-0.2486**
H	**1.0179**	**4.5439**	**2.1751**
H	**0.2945**	**4.6833**	**0.5510**
H	**0.0631**	**3.1970**	**1.5225**
H	**2.9898**	**2.9053**	**2.5574**
H	**2.0051**	**1.5914**	**1.8969**
H	**3.6140**	**1.9359**	**1.1950**
H	**1.0181**	**-4.5440**	**2.1740**
H	**0.0636**	**-3.1967**	**1.5217**
H	**0.2945**	**-4.6828**	**0.5499**
H	**2.9903**	**-2.9061**	**2.5566**
H	**3.6151**	**-1.9367**	**1.1945**
H	**2.0062**	**-1.5917**	**1.8963**
H	**3.3248**	**-5.0258**	**1.3650**
H	**2.6510**	**-5.3277**	**-0.2505**
H	**4.0090**	**-4.1872**	**-0.0492**
H	**-0.6056**	**-0.9056**	**5.0748**
H	**-0.6063**	**0.9043**	**5.0749**
H	**-2.0852**	**-0.0011**	**4.6712**

Model 25

97

Cd	**0.0000**	**0.0001**	**0.0006**
O	**-2.1817**	**-0.4271**	**-0.3549**
O	**-0.6090**	**2.0056**	**-0.8253**
O	**-0.1424**	**-0.9887**	**-2.2360**
O	**2.1820**	**0.4272**	**0.3552**
O	**0.6092**	**-2.0051**	**0.8268**
O	**0.1434**	**0.9893**	**2.2371**
H	**-1.1118**	**-1.0280**	**-2.1233**
H	**-4.7549**	**4.2587**	**-1.3632**
H	**-4.4578**	**4.4560**	**0.3784**
H	**-5.9777**	**3.7104**	**-0.1872**
H	**-2.6748**	**4.5331**	**-0.9747**
H	**-1.2137**	**4.2679**	**-1.9333**
H	**-0.9510**	**3.4941**	**1.7743**
H	**-2.3058**	**4.6555**	**1.7114**
H	**-0.7021**	**5.1846**	**2.2684**
H	**1.0000**	**4.9874**	**-1.1055**
H	**0.9529**	**3.6360**	**0.0474**
H	**1.2576**	**5.2987**	**0.6302**
H	**-0.8997**	**6.7132**	**-1.1627**
H	**-0.5341**	**7.0447**	**0.5478**
H	**-2.1975**	**6.6400**	**0.0562**
H	**-3.3104**	**-2.2202**	**0.1519**
H	**-4.5661**	**-4.3242**	**0.5114**
H	**-7.0598**	**-4.3014**	**0.6694**
H	**-8.2754**	**-2.1250**	**0.4639**
H	**-7.0049**	**-0.0141**	**0.1042**
H	**1.2589**	**-0.2156**	**-3.4819**
H	**-0.1866**	**0.8082**	**-3.3044**
H	**-0.1555**	**-0.3011**	**-5.5664**
H	**-1.5394**	**-0.8923**	**-4.6161**
H	**-0.0799**	**-1.9089**	**-4.7885**
H	**1.1128**	**1.0285**	**2.1238**
H	**4.7553**	**-4.2589**	**1.3619**
H	**4.4565**	**-4.4563**	**-0.3795**
H	**5.9771**	**-3.7110**	**0.1847**
H	**2.6747**	**-4.5330**	**0.9753**
H	**1.2144**	**-4.2673**	**1.9350**
H	**0.9492**	**-3.4942**	**-1.7726**
H	**2.3035**	**-4.6562**	**-1.7105**
H	**0.6992**	**-5.1847**	**-2.2662**
H	**-1.0002**	**-4.9865**	**1.1090**
H	**-0.9537**	**-3.6354**	**-0.0442**
H	**-1.2592**	**-5.2982**	**-0.6264**
H	**0.8992**	**-6.7127**	**1.1651**
H	**0.5322**	**-7.0445**	**-0.5450**
H	**2.1961**	**-6.6401**	**-0.0547**
H	**3.3106**	**2.2200**	**-0.1526**
H	**4.5663**	**4.3238**	**-0.5136**
H	**7.0599**	**4.3006**	**-0.6737**
H	**8.2752**	**2.1240**	**-0.4689**
H	**7.0048**	**0.0134**	**-0.1078**
H	**-1.2573**	**0.2162**	**3.4837**
H	**0.1881**	**-0.8077**	**3.3054**
H	**0.1583**	**0.3016**	**5.5674**
H	**1.5417**	**0.8927**	**4.6163**
H	**0.0825**	**1.9094**	**4.7896**
N	**-4.4034**	**0.2505**	**-0.1018**
N	**-5.1486**	**1.4180**	**-0.1139**
N	**4.4033**	**-0.2508**	**0.1004**
N	**5.1484**	**-1.4184**	**0.1120**
C	**-3.0639**	**0.4993**	**-0.3107**
C	**-2.9497**	**1.9313**	**-0.4629**
C	**-4.3127**	**2.4069**	**-0.3229**
C	**-4.8984**	**3.7871**	**-0.3775**
C	**-1.7211**	**2.6093**	**-0.7251**
C	**-0.8258**	**4.9210**	**0.1056**
C	**-1.6650**	**4.1125**	**-0.9379**
C	**-1.2222**	**4.5363**	**1.5435**
C	**0.6841**	**4.6917**	**-0.0907**
C	**-1.1341**	**6.4128**	**-0.1276**
C	**-5.0827**	**-0.9827**	**0.1018**
C	**-4.3940**	**-2.2027**	**0.2186**
C	**-5.1140**	**-3.3831**	**0.4214**
C	**-6.5076**	**-3.3727**	**0.5108**
C	**-7.1853**	**-2.1551**	**0.3957**
C	**-6.4859**	**-0.9660**	**0.1925**
C	**0.1602**	**-0.2328**	**-3.4265**
C	**-0.4372**	**-0.8742**	**-4.6678**
C	**3.0640**	**-0.4993**	**0.3105**
C	**2.9497**	**-1.9313**	**0.4629**
C	**4.3125**	**-2.4072**	**0.3218**
C	**4.8980**	**-3.7875**	**0.3760**
C	**1.7211**	**-2.6091**	**0.7261**
C	**0.8247**	**-4.9208**	**-0.1035**
C	**1.6649**	**-4.1122**	**0.9392**
C	**1.2201**	**-4.5365**	**-1.5417**
C	**-0.6850**	**-4.6911**	**0.0940**
C	**1.1328**	**-6.4126**	**0.1298**
C	**5.0827**	**0.9822**	**-0.1039**
C	**4.3941**	**2.2024**	**-0.2203**
C	**5.1141**	**3.3826**	**-0.4239**
C	**6.5076**	**3.3720**	**-0.5145**
C	**7.1852**	**2.1543**	**-0.3998**
C	**6.4858**	**0.9653**	**-0.1958**
C	**-0.1585**	**0.2334**	**3.4276**
C	**0.4396**	**0.8747**	**4.6687**

Model 26

99

Cd	**-0.1177**	**-0.0295**	**-0.1107**
C	**-3.2156**	**3.2948**	**1.6414**
C	**-3.5008**	**2.9521**	**0.1560**
C	**-2.9520**	**4.0549**	**-0.7705**
C	**-3.4970**	**5.4371**	**-0.3879**
C	**-3.1988**	**5.7723**	**1.0792**
C	**-3.7428**	**4.6864**	**2.0165**
C	**-2.8852**	**1.5909**	**-0.1532**
C	**-0.0376**	**-0.2615**	**3.3526**
C	**0.3017**	**0.4666**	**4.6434**
C	**2.8740**	**0.7987**	**-0.0488**
C	**3.4204**	**-0.5389**	**-0.1098**
C	**4.7969**	**-0.3279**	**-0.5241**
C	**2.6466**	**-1.6901**	**0.2624**
C	**3.9443**	**3.0677**	**-0.4218**
C	**5.1830**	**3.6995**	**-0.6303**
C	**5.2540**	**5.0907**	**-0.6925**
C	**4.1036**	**5.8724**	**-0.5486**
C	**2.8759**	**5.2394**	**-0.3431**
C	**2.7825**	**3.8465**	**-0.2782**
C	**5.8970**	**-1.2687**	**-0.9221**
C	**3.2127**	**-3.0707**	**0.6156**
C	**3.6692**	**-3.9129**	**-0.5965**
C	**4.0457**	**-5.3352**	**-0.1540**
C	**5.1008**	**-5.3222**	**0.9611**
C	**4.6350**	**-4.4880**	**2.1628**
C	**4.2571**	**-3.0567**	**1.7520**
C	**-0.2261**	**0.5402**	**-3.4791**
C	**-0.5413**	**-0.0375**	**-4.8490**
C	**-3.1049**	**-0.9293**	**-0.3024**
C	**-5.0632**	**0.1485**	**0.1402**
C	**-3.6547**	**0.3888**	**-0.1004**
C	**-4.2010**	**-3.2162**	**-0.3012**
C	**-5.4520**	**-3.8580**	**-0.3028**
C	**-5.5225**	**-5.2457**	**-0.4197**
C	**-4.3598**	**-6.0134**	**-0.5372**
C	**-3.1199**	**-5.3706**	**-0.5327**
C	**-3.0269**	**-3.9813**	**-0.4150**
C	**-6.1948**	**1.0909**	**0.4249**
O	**-1.6456**	**1.6043**	**-0.4140**
O	**-0.1689**	**0.6489**	**2.2462**
O	**1.7082**	**1.2271**	**0.2629**
O	**1.3873**	**-1.6280**	**0.3991**
O	**-0.0657**	**-0.4962**	**-2.4904**
O	**-1.9111**	**-1.3180**	**-0.5537**
N	**5.0640**	**0.9496**	**-0.6734**
N	**3.9121**	**1.6465**	**-0.3692**
N	**-4.1664**	**-1.8002**	**-0.1761**
N	**-5.3500**	**-1.1310**	**0.0885**
H	**-0.9103**	**-0.9771**	**-2.3918**
H	**-2.0595**	**-3.4878**	**-0.4110**
H	**-2.2004**	**-5.9545**	**-0.6199**
H	**-4.4204**	**-7.0999**	**-0.6297**
H	**-6.5021**	**-5.7299**	**-0.4198**
H	**-6.3511**	**-3.2528**	**-0.2075**
H	**0.7346**	**1.0766**	**-3.4904**
H	**-1.0043**	**1.2525**	**-3.1530**
H	**-0.6057**	**0.7682**	**-5.5987**
H	**-1.5085**	**-0.5687**	**-4.8451**
H	**0.2405**	**-0.7462**	**-5.1643**
H	**0.6890**	**1.0899**	**2.0901**
H	**6.1578**	**-1.9962**	**-0.1418**
H	**5.6279**	**-1.8359**	**-1.8278**
H	**6.7876**	**-0.6678**	**-1.1514**
H	**1.8248**	**3.3604**	**-0.1176**
H	**1.9659**	**5.8338**	**-0.2310**
H	**4.1644**	**6.9618**	**-0.5971**
H	**6.0721**	**3.0832**	**-0.7452**
H	**-1.0145**	**-0.7623**	**3.4309**
H	**0.7159**	**-1.0346**	**3.1186**
H	**0.3460**	**-0.2441**	**5.4851**
H	**1.2842**	**0.9642**	**4.5737**
H	**-0.4564**	**1.2320**	**4.8721**
H	**2.3217**	**-3.5831**	**1.0158**
H	**5.1633**	**-2.5116**	**1.4465**
H	**3.8480**	**-2.5099**	**2.6185**
H	**5.4179**	**-4.4607**	**2.9392**
H	**3.7558**	**-4.9770**	**2.6227**
H	**6.0451**	**-4.9010**	**0.5667**
H	**5.3308**	**-6.3528**	**1.2800**
H	**4.4097**	**-5.9124**	**-1.0206**
H	**3.1398**	**-5.8545**	**0.2106**
H	**4.5340**	**-3.4495**	**-1.0926**
H	**2.8566**	**-3.9476**	**-1.3412**
H	**-4.5900**	**2.9031**	**0.0239**
H	**-1.8521**	**4.0525**	**-0.7067**
H	**-3.2066**	**3.8199**	**-1.8183**
H	**-3.0664**	**6.2054**	**-1.0521**
H	**-4.5913**	**5.4631**	**-0.5516**
H	**-2.1044**	**5.8566**	**1.2171**
H	**-3.6253**	**6.7546**	**1.3439**
H	**-3.4797**	**4.9135**	**3.0636**
H	**-4.8482**	**4.6847**	**1.9670**
H	**-2.1250**	**3.2436**	**1.8056**
H	**-3.6644**	**2.5269**	**2.2940**
H	**6.2241**	**5.5666**	**-0.8548**
H	**-6.3753**	**1.7844**	**-0.4126**
H	**-7.1066**	**0.4987**	**0.5834**
H	**-6.0117**	**1.6981**	**1.3255**

OP3 Protocol

Model 1

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Cd	-0.052506	0.074621	0.031076
C	0.913429	1.375913	-2.869708
N	0.102718	0.490065	-2.299471
C	-0.595409	-0.120093	-3.327820
C	-0.192146	0.411577	-4.529355
N	0.771466	1.366908	-4.225993
O	-1.861842	-1.313288	-0.399597
C	-3.077198	-0.944385	-0.396014
C	-3.710257	0.318968	-0.047945
C	-5.122001	0.103465	-0.304898
N	-5.362650	-1.118750	-0.734258
N	-4.128869	-1.787300	-0.767746
C	-3.017589	1.488060	0.382127
C	-3.757156	2.675162	0.959777
C	-4.574031	2.547694	2.094919
C	-5.147051	3.678619	2.688946
C	-4.925458	4.948002	2.143292
C	-4.110409	5.083619	1.011263
C	-3.516544	3.957305	0.435361
C	-4.104613	-3.142542	-1.190480
C	-6.292890	1.047944	-0.232658
C	1.505180	2.201810	-5.180874
O	1.860666	1.405115	0.235845
C	3.051401	0.986193	0.098850
C	3.610835	-0.355114	0.023611
C	5.030397	-0.149492	-0.194617
N	5.341710	1.130668	-0.233888
N	4.150934	1.843494	-0.023422
C	2.849933	-1.559394	0.091052
O	1.579639	-1.620793	0.032780
C	4.202762	3.262428	-0.016735
C	6.141491	-1.133720	-0.450622
C	3.518267	-2.905356	0.268700
C	3.185114	-3.956593	-0.604185
C	3.714347	-5.235450	-0.410917
C	4.556086	-5.491173	0.680276
C	4.869274	-4.457915	1.570717
C	4.361223	-3.170097	1.360591
N	-0.175707	-0.302874	2.379139
C	0.179264	-1.431659	2.983128
N	-0.059217	-1.365499	4.325221
C	-0.598664	-0.110186	4.581786
C	-0.664273	0.532623	3.368628
C	0.193421	-2.422558	5.307281
O	-1.753543	1.642021	0.345556
H	1.600047	2.025760	-2.346249
H	-0.493754	0.206068	-5.546143
H	-1.329748	-0.887546	-3.132260
H	2.191434	2.848624	-4.630158
H	2.082776	1.575479	-5.868484
H	0.810970	2.824622	-5.754399
H	-1.028291	1.523872	3.140750
H	-0.876384	0.199651	5.578767
H	0.604119	-2.297130	2.494278
H	0.891866	-2.071448	6.073921
H	-0.742396	-2.732050	5.784224
H	0.631312	-3.282546	4.796021
H	-7.147366	0.579102	-0.730043
H	-6.576749	1.276215	0.800576
H	-6.073341	2.002341	-0.723972
H	-4.744698	1.562798	2.523132
H	-5.765023	3.567249	3.577147
H	-5.377226	5.825903	2.599856
H	-3.930097	6.067988	0.584803
H	-2.857808	4.061206	-0.423154
H	7.016794	-0.583106	-0.808602
H	6.425363	-1.681768	0.454599
H	5.856517	-1.879081	-1.201532
H	4.605424	-2.369090	2.054562
H	5.509780	-4.652559	2.428152
H	4.958583	-6.489443	0.837719
H	3.463696	-6.035076	-1.104564
H	2.506411	-3.760876	-1.430569
C	-2.923557	-3.911434	-1.161173
C	-2.954107	-5.245241	-1.581735
C	-4.139545	-5.835650	-2.031862
C	-5.310916	-5.068537	-2.056555
C	-5.301441	-3.735894	-1.642220
H	-2.003357	-3.463609	-0.812848
H	-2.034465	-5.825753	-1.550977
H	-4.152278	-6.873696	-2.355434
H	-6.244420	-5.508335	-2.401172
H	-6.206183	-3.140750	-1.656903
C	3.085702	4.045866	0.337406
C	3.189170	5.441032	0.336255
C	4.386270	6.077544	-0.008056
C	5.494939	5.294799	-0.353910
C	5.411715	3.901520	-0.361182
H	2.158686	3.561907	0.612039
H	2.319539	6.031323	0.616820
H	4.456980	7.162577	-0.001736
H	6.437068	5.769742	-0.619283
H	6.268978	3.292446	-0.620881

Model 2

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Cd	**0.073478**	**0.271888**	**0.116940**
C	**-4.688701**	**-0.741243**	**2.083432**
C	**-4.379889**	**-0.937536**	**0.725679**
C	**-5.052691**	**-1.945736**	**0.016834**
C	**-6.022072**	**-2.734899**	**0.648329**
C	**-6.343385**	**-2.512842**	**1.992020**
C	**-5.675007**	**-1.509944**	**2.707468**
C	**-3.234022**	**-0.160006**	**0.110835**
C	**-3.399207**	**0.597737**	**-1.082954**
C	**-2.303234**	**1.215246**	**-1.826967**
N	**-2.912742**	**1.832947**	**-2.895703**
N	**-4.301916**	**1.715601**	**-2.878644**
C	**-4.595887**	**0.986021**	**-1.814447**
O	**-1.040576**	**1.268326**	**-1.648528**
C	**-2.256794**	**2.558560**	**-3.966298**
C	**-6.054356**	**0.754543**	**-1.516840**
O	**-2.138082**	**-0.277306**	**0.748889**
N	**0.109069**	**-1.880390**	**-0.945287**
C	**-0.586467**	**-2.933301**	**-0.533214**
N	**-0.320814**	**-4.030015**	**-1.302497**
C	**0.604975**	**-3.637705**	**-2.262996**
C	**0.859343**	**-2.307345**	**-2.026553**
C	**-0.894448**	**-5.367193**	**-1.139534**
O	**2.268915**	**0.563358**	**-0.637148**
C	**3.357566**	**0.095383**	**-0.167808**
C	**4.511303**	**0.146521**	**-1.147218**
C	**5.183146**	**-1.017674**	**-1.553158**
C	**6.160799**	**-0.963015**	**-2.554079**
C	**6.491314**	**0.259927**	**-3.148397**
C	**5.823856**	**1.426304**	**-2.750487**
C	**4.829397**	**1.366055**	**-1.770451**
C	**3.509488**	**-0.446496**	**1.139345**
C	**2.406885**	**-0.702603**	**2.063306**
N	**3.009114**	**-1.204250**	**3.194156**
N	**4.399962**	**-1.244886**	**3.103546**
C	**4.701629**	**-0.807026**	**1.891821**
O	**1.141780**	**-0.546346**	**1.985915**
C	**6.161917**	**-0.689779**	**1.541818**
C	**2.347935**	**-1.625042**	**4.413956**
N	**-0.024913**	**2.394156**	**1.213336**
C	**0.485770**	**2.747425**	**2.449711**
C	**0.182918**	**4.062896**	**2.710604**
N	**-0.529628**	**4.520721**	**1.607461**
C	**-0.626279**	**3.476135**	**0.733363**
C	**-1.075464**	**5.866503**	**1.419533**
H	**-1.129974**	**3.538509**	**-0.220612**
H	**0.401415**	**4.701367**	**3.554383**
H	**1.026998**	**2.035643**	**3.055263**
H	**-1.603852**	**5.903221**	**0.464336**
H	**-1.780022**	**6.107894**	**2.222236**
H	**-0.270588**	**6.609119**	**1.409722**
H	**1.524935**	**-1.637001**	**-2.550977**
H	**0.984295**	**-4.325132**	**-3.005156**
H	**-1.280803**	**-2.941522**	**0.295440**
H	**-1.427528**	**-5.667683**	**-2.047658**
H	**-0.107477**	**-6.097766**	**-0.924183**
H	**-1.599210**	**-5.349991**	**-0.305294**
H	**1.272311**	**-1.509261**	**4.264178**
H	**2.580010**	**-2.674205**	**4.632583**
H	**2.672541**	**-1.009146**	**5.261943**
H	**6.749184**	**-0.842080**	**2.452846**
H	**6.474055**	**-1.435635**	**0.801874**
H	**6.401723**	**0.294761**	**1.124378**
H	**4.924718**	**-1.970154**	**-1.096703**
H	**6.662235**	**-1.875486**	**-2.869495**
H	**7.255953**	**0.303930**	**-3.920946**
H	**6.071328**	**2.379773**	**-3.212320**
H	**4.285485**	**2.262326**	**-1.482988**
H	**-2.478660**	**2.094800**	**-4.934794**
H	**-2.595437**	**3.601874**	**-3.990906**
H	**-1.181283**	**2.522019**	**-3.779903**
H	**-6.647451**	**1.401957**	**-2.170410**
H	**-6.356573**	**-0.283630**	**-1.695845**
H	**-6.297954**	**0.983241**	**-0.473089**
H	**-4.804432**	**-2.121601**	**-1.027177**
H	**-6.526306**	**-3.520918**	**0.090183**
H	**-7.102734**	**-3.119435**	**2.480594**
H	**-5.915576**	**-1.335092**	**3.753946**
H	**-4.143524**	**0.014034**	**2.643918**

Model 3

113

Cd	**-0.033697**	**-0.218769**	**-0.175439**
C	**-2.975376**	**0.443171**	**-1.816693**
N	**-2.189041**	**0.667876**	**-0.698919**
C	**-2.974626**	**1.257055**	**0.195788**
N	**-4.237941**	**1.429010**	**-0.295109**
C	**-4.248355**	**0.905212**	**-1.583463**
O	**0.135370**	**1.575085**	**1.338823**
C	**0.765666**	**2.676687**	**1.248523**
C	**0.494911**	**3.636980**	**2.384571**
C	**0.592754**	**3.177382**	**3.709909**
C	**0.262221**	**4.015238**	**4.778347**
C	**-0.205974**	**5.313772**	**4.535242**
C	**-0.333029**	**5.769708**	**3.218233**
C	**0.025012**	**4.939554**	**2.149312**
C	**-5.401686**	**1.921598**	**0.476158**
O	**1.139614**	**1.275700**	**-1.520650**
C	**1.754565**	**2.292925**	**-1.072821**
N	**2.754833**	**2.956359**	**-1.792730**
N	**3.311865**	**4.011087**	**-1.052517**
C	**2.654297**	**4.061099**	**0.089397**
C	**1.643865**	**3.024501**	**0.178331**
C	**3.297898**	**2.662122**	**-3.071199**
C	**4.482098**	**3.312284**	**-3.475435**
C	**5.035031**	**3.045214**	**-4.729007**
C	**4.428099**	**2.131990**	**-5.600438**
C	**3.251005**	**1.491609**	**-5.198610**
C	**2.679147**	**1.747862**	**-3.947735**
C	**3.099510**	**5.092002**	**1.093264**
O	**-0.521240**	**-1.954411**	**-1.655250**
C	**-1.247530**	**-2.988435**	**-1.499063**
C	**-1.733528**	**-3.466932**	**-0.248215**
C	**-1.592462**	**-2.772788**	**1.024151**
N	**-2.223265**	**-3.598399**	**1.959921**
N	**-2.692573**	**-4.783166**	**1.369739**
C	**-2.412643**	**-4.705710**	**0.084823**
O	**-1.037034**	**-1.673705**	**1.335546**
C	**-2.772060**	**-5.894800**	**-0.766689**
C	**-2.436928**	**-3.405878**	**3.350297**
C	**-2.022787**	**-2.233230**	**4.014408**
C	**-2.269525**	**-2.087596**	**5.383707**
C	**-2.921262**	**-3.087542**	**6.112961**
C	**-3.329955**	**-4.251140**	**5.449351**
C	**-3.094182**	**-4.415683**	**4.083614**
N	**2.082511**	**-1.184545**	**0.317627**
C	**3.215977**	**-0.948617**	**-0.335473**
N	**4.233329**	**-1.716311**	**0.153701**
C	**3.703109**	**-2.490424**	**1.180388**
C	**2.375007**	**-2.149314**	**1.268117**
C	**5.613773**	**-1.763080**	**-0.375191**
C	**-1.582640**	**-3.693663**	**-2.797148**
C	**-2.905137**	**-3.790857**	**-3.257733**
C	**-3.181207**	**-4.339201**	**-4.516133**
C	**-2.139018**	**-4.812932**	**-5.320724**
C	**-0.816176**	**-4.717011**	**-4.868702**
C	**-0.539520**	**-4.146037**	**-3.623220**
H	**3.336969**	**-0.254650**	**-1.154688**
H	**4.308942**	**-3.179930**	**1.749154**
H	**1.617251**	**-2.524412**	**1.940225**
H	**-2.576274**	**-0.030080**	**-2.701957**
H	**-5.131613**	**0.930401**	**-2.203890**
H	**-2.674265**	**1.561985**	**1.188077**
H	**-3.079939**	**-6.711948**	**-0.107294**
H	**-3.595226**	**-5.675641**	**-1.455561**
H	**-1.924089**	**-6.227543**	**-1.375599**
H	**-3.717112**	**-3.421918**	**-2.635460**
H	**-4.209381**	**-4.395643**	**-4.866779**
H	**-2.353690**	**-5.245921**	**-6.295193**
H	**-0.000346**	**-5.077827**	**-5.491292**
H	**0.487879**	**-4.042888**	**-3.282852**
H	**4.040405**	**5.530420**	**0.746893**
H	**2.366211**	**5.897417**	**1.210634**
H	**3.253439**	**4.651551**	**2.084736**
H	**-0.077995**	**5.294001**	**1.126449**
H	**-0.710910**	**6.770564**	**3.021826**
H	**-0.476436**	**5.961256**	**5.366252**
H	**0.360210**	**3.654060**	**5.799722**
H	**0.926765**	**2.158986**	**3.891062**
H	**-1.518035**	**-1.455288**	**3.458901**
H	**-1.944447**	**-1.176021**	**5.880780**
H	**-3.107381**	**-2.963997**	**7.177137**
H	**-3.838508**	**-5.041923**	**5.996781**
H	**-3.411259**	**-5.313439**	**3.567458**
H	**1.765293**	**1.253854**	**-3.647682**
H	**2.759571**	**0.786294**	**-5.865152**
H	**4.862030**	**1.928761**	**-6.576513**
H	**5.947445**	**3.558487**	**-5.024903**
H	**4.944292**	**4.023462**	**-2.801523**
C	**-6.311541**	**2.853521**	**-0.306604**
H	**-5.974001**	**1.057383**	**0.831536**
H	**-4.993499**	**2.430446**	**1.355012**
C	**6.688816**	**-1.576254**	**0.684612**
H	**5.758773**	**-2.721690**	**-0.885395**
H	**5.677432**	**-0.974755**	**-1.131548**
C	**-7.608302**	**2.445091**	**-0.653447**
C	**-8.461909**	**3.300709**	**-1.361666**
C	**-8.023559**	**4.576247**	**-1.730551**
C	**-6.730377**	**4.993486**	**-1.387263**
C	**-5.880898**	**4.138663**	**-0.679163**
H	**-7.954710**	**1.453520**	**-0.365823**
H	**-9.464364**	**2.970031**	**-1.622481**
H	**-8.683899**	**5.243121**	**-2.280003**
H	**-6.385554**	**5.985457**	**-1.668941**
H	**-4.877125**	**4.469136**	**-0.417165**
C	**7.585620**	**-2.616391**	**0.970294**
C	**8.592390**	**-2.448789**	**1.930015**
C	**8.708268**	**-1.235778**	**2.615751**
C	**7.816640**	**-0.191047**	**2.336492**
C	**6.815224**	**-0.358840**	**1.376049**
H	**7.500085**	**-3.562488**	**0.437560**
H	**9.280879**	**-3.263839**	**2.139643**
H	**9.487998**	**-1.102385**	**3.362084**
H	**7.903973**	**0.755438**	**2.864584**
H	**6.127696**	**0.458098**	**1.164190**

Model 4

99

Cd	0.209861	-0.070071	-0.054993
C	-2.586656	-3.867291	-1.856157
C	-2.838856	-4.376461	-0.565632
C	-3.849832	-5.344377	-0.393031
C	-4.593403	-5.785251	-1.489108
C	-4.351800	-5.276292	-2.771362
C	-3.345539	-4.319693	-2.940917
N	-2.100314	-3.943678	0.567163
C	-1.209751	-2.868374	0.694335
C	-0.814793	-2.870731	2.091706
C	-1.532876	-3.986404	2.673154
N	-2.285343	-4.610505	1.787807
O	-0.903483	-2.110366	-0.276501
O	0.636836	-0.971860	2.088524
C	0.077690	-1.934540	2.699594
C	0.428481	-2.050264	4.187679
C	-1.543185	-4.521291	4.081519
N	-1.954068	0.787651	0.504269
C	-3.103816	0.140965	0.343826
N	-4.152225	0.873694	0.821141
C	-3.625771	2.061412	1.318775
C	-2.268843	1.992364	1.112745
O	0.123968	0.719530	-2.249969
C	0.381485	1.873064	-2.717503
C	0.899427	2.964184	-1.955272
C	1.197815	2.938229	-0.534105
N	1.688193	4.216010	-0.240870
N	1.708534	5.035660	-1.379349
C	1.247588	4.306333	-2.375787
O	1.072971	2.029854	0.347017
C	1.169914	4.965207	-3.728483
C	2.128818	4.760495	0.994658
C	2.206275	3.981687	2.167270
C	2.647327	4.565061	3.359832
C	3.017566	5.912772	3.413365
C	2.941629	6.681928	2.245459
C	2.502617	6.119383	1.045887
N	2.295723	-1.078437	-0.653266
C	2.836118	-1.246690	-1.917016
C	4.021548	-1.935402	-1.822658
N	4.212015	-2.189308	-0.468642
C	3.141573	-1.655069	0.191705
C	0.098957	2.038472	-4.215197
H	-3.217243	-0.838388	-0.097699
H	-4.251860	2.831240	1.745053
H	-1.505203	2.717835	1.352347
H	2.337894	-0.861608	-2.794448
H	4.737903	-2.246067	-2.568739
H	3.012281	-1.710920	1.262792
H	1.527555	5.994852	-3.634720
H	1.789799	4.450369	-4.472235
H	0.144135	4.988510	-4.115375
H	-2.229178	-5.372320	4.126269
H	-0.549756	-4.862716	4.396879
H	-1.875431	-3.767789	4.805333
H	1.924060	2.938755	2.133943
H	2.700688	3.950120	4.255875
H	3.359199	6.356015	4.345808
H	3.225736	7.732003	2.264235
H	2.444424	6.711835	0.141030
H	-1.806211	-3.132540	-1.997041
H	-3.137053	-3.918267	-3.930358
H	-4.934211	-5.622569	-3.621831
H	-5.368291	-6.533438	-1.336390
H	-4.031519	-5.739256	0.599285
H	1.161759	-1.276170	4.426539
H	-0.458709	-1.900307	4.813523
H	0.843261	-3.033590	4.434217
H	1.007173	2.301780	-4.768703
H	-0.291092	1.091157	-4.595162
H	-0.638844	2.827638	-4.397318
C	-5.557988	0.423673	0.888231
H	-5.588759	-0.552718	0.394451
H	-5.822513	0.265944	1.939560
C	-6.553449	1.377337	0.244620
C	-7.574232	1.954522	1.014205
C	-8.517308	2.807936	0.426796
C	-8.445350	3.093085	-0.940062
C	-7.428157	2.521467	-1.716661
C	-6.489876	1.668543	-1.129063
H	-7.635470	1.734045	2.079053
H	-9.303187	3.246913	1.036764
H	-9.175689	3.755190	-1.399347
H	-7.368370	2.738177	-2.780603
H	-5.702808	1.228758	-1.739313
C	5.307379	-2.966839	0.143725
C	6.703185	-2.463072	-0.195166
H	5.139339	-2.927543	1.225267
H	5.207590	-4.013841	-0.163141
C	7.641572	-3.333761	-0.768859
C	8.942645	-2.897242	-1.050480
C	9.315052	-1.580468	-0.763360
C	8.382762	-0.702916	-0.193105
C	7.086380	-1.141281	0.091294
H	7.355775	-4.359832	-0.996256
H	9.658776	-3.583966	-1.495410
H	10.323436	-1.237555	-0.983091
H	8.665414	0.322852	0.030580
H	6.367986	-0.450541	0.529332

Model 5

99

Cd	-0.101089	0.117692	0.220897
C	-2.964090	-1.100274	1.622134
N	-2.382672	-0.510250	0.512513
C	-3.377144	-0.199911	-0.309976
N	-4.584019	-0.566824	0.216395
C	-4.327741	-1.141272	1.457923
O	0.713232	-1.946262	-0.580317
C	1.199257	-2.954387	0.021755
C	1.476125	-4.141912	-0.872012
C	2.136771	-3.934715	-2.096327
C	2.338952	-4.994166	-2.984349
C	1.849147	-6.271062	-2.677822
C	1.161235	-6.479202	-1.477068
C	0.984157	-5.423317	-0.575462
C	-5.906895	-0.278161	-0.372344
N	2.169291	0.904522	0.210025
C	3.233906	0.195039	0.567538
N	4.366569	0.959102	0.547120
C	3.986536	2.238420	0.153869
C	2.628843	2.184962	-0.051425
C	5.711954	0.520700	0.969975
O	-0.634779	2.347698	0.819045
C	-1.121657	3.307394	0.142318
C	-1.215880	3.311273	-1.282624
C	-0.995282	2.134501	-2.117761
N	-1.154975	2.586201	-3.408023
N	-1.402582	3.955724	-3.481754
C	-1.451687	4.388096	-2.231074
O	-0.746094	0.909613	-1.854919
C	-1.648585	5.866077	-2.016023
C	-1.013714	1.803618	-4.621444
O	0.219675	-0.979005	2.253555
C	0.964809	-2.006767	2.377130
C	1.469428	-2.991802	1.424365
C	2.273890	-3.896198	2.229227
N	2.273756	-3.543316	3.506024
N	1.459430	-2.415913	3.595668
C	3.136029	-5.066440	1.832220
C	1.229137	-1.781280	4.879705
C	-1.610517	4.471576	0.975495
C	-2.910120	4.986069	0.840787
C	-3.373762	5.985952	1.703632
C	-2.536293	6.497481	2.701150
C	-1.238988	5.987346	2.845737
C	-0.787602	4.969859	2.001386
H	3.230901	-0.847784	0.854686
H	4.702887	3.038440	0.039858
H	1.959689	2.970251	-0.370870
H	-2.358472	-1.444781	2.447168
H	-5.119128	-1.529068	2.082160
H	-3.264509	0.282935	-1.269833
H	-0.779126	0.778381	-4.327101
H	-1.944738	1.819599	-5.201091
H	-0.204594	2.204467	-5.243429
H	-1.536955	6.374135	-2.979018
H	-2.641552	6.101141	-1.616079
H	-0.916151	6.275061	-1.310850
H	-3.566296	4.585712	0.072032
H	-4.388957	6.362421	1.598487
H	-2.893712	7.279591	3.367460
H	-0.585449	6.374141	3.624670
H	0.203169	4.543272	2.134583
H	0.679227	-2.452367	5.551119
H	2.183265	-1.516691	5.350093
H	0.641640	-0.878178	4.700680
H	3.787557	-5.319863	2.674510
H	2.543074	-5.952396	1.578467
H	3.756082	-4.838773	0.957490
H	0.439979	-5.585552	0.351476
H	0.758461	-7.462148	-1.243064
H	1.993389	-7.093473	-3.375139
H	2.865688	-4.823203	-3.920780
H	2.477399	-2.933251	-2.346582
C	-6.833306	-1.481874	-0.462588
H	-6.386350	0.511951	0.216519
H	-5.713707	0.130443	-1.369689
C	-8.072385	-1.465459	0.194880
C	-8.951463	-2.551414	0.091526
C	-8.595390	-3.667946	-0.670962
C	-7.358354	-3.694036	-1.329522
C	-6.484016	-2.608378	-1.227472
H	-8.354351	-0.597977	0.789952
H	-9.908652	-2.523216	0.606705
H	-9.275129	-4.512955	-0.752994
H	-7.076137	-4.559475	-1.924318
H	-5.523689	-2.638350	-1.739422
C	6.812347	0.826162	-0.035616
H	5.948750	0.991312	1.930722
H	5.640171	-0.557789	1.144773
C	7.909055	1.615374	0.341028
C	8.944824	1.879497	-0.564641
C	8.889487	1.357730	-1.860580
C	7.796638	0.569324	-2.246139
C	6.766608	0.303469	-1.339715
H	7.956113	2.025234	1.348967
H	9.788446	2.492752	-0.257199
H	9.690365	1.562972	-2.567076
H	7.748308	0.160568	-3.252612
H	5.919965	-0.307461	-1.648204

Model 6
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Cd	**0.000033**	**-0.001341**	**0.002114**
C	**-2.867055**	**2.748011**	**-2.481280**
C	**-1.549493**	**2.366635**	**-2.133650**
N	**-1.589281**	**1.367469**	**-1.226872**
N	**-2.918861**	**1.096635**	**-0.982330**
C	**-3.694494**	**1.922383**	**-1.732667**
N	**1.589918**	**-1.366446**	**1.228932**
N	**2.919259**	**-1.096875**	**0.982234**
C	**3.695260**	**-1.927775**	**1.726509**
C	**2.868206**	**-2.755491**	**2.473178**
C	**1.550454**	**-2.369846**	**2.130928**
B	**-3.396398**	**0.000525**	**0.008717**
N	**-2.916184**	**0.309693**	**1.452624**
N	**-1.586054**	**0.383569**	**1.807394**
C	**-1.543660**	**0.667751**	**3.126230**
C	**-2.860232**	**0.779722**	**3.632655**
C	**-3.689827**	**0.546670**	**2.544425**
B	**3.396180**	**0.000375**	**-0.007759**
N	**2.918214**	**1.405591**	**0.448300**
N	**1.588594**	**1.751289**	**0.563860**
C	**1.548380**	**3.035215**	**0.978534**
C	**2.865805**	**3.527956**	**1.133322**
C	**3.693587**	**2.468336**	**0.788844**
N	**-1.589390**	**-1.751179**	**-0.561191**
N	**-2.919001**	**-1.405163**	**-0.446917**
C	**-3.694218**	**-2.465578**	**-0.794828**
C	**-2.866308**	**-3.524113**	**-1.142524**
C	**-1.548959**	**-3.033313**	**-0.981585**
N	**1.585831**	**-0.385633**	**-1.805775**
N	**2.916080**	**-0.308074**	**-1.451969**
C	**3.689605**	**-0.538049**	**-2.545267**
C	**2.859928**	**-0.770377**	**-3.633620**
C	**1.543421**	**-0.665417**	**-3.125649**
H	**-4.597018**	**0.000963**	**0.010097**
H	**4.596779**	**0.000563**	**-0.009313**
C	**0.254163**	**-2.933268**	**2.644360**
H	**4.773283**	**-1.870125**	**1.670649**
H	**3.169087**	**-3.529244**	**3.167325**
H	**-4.772338**	**-2.389957**	**-0.770521**
H	**-3.166348**	**-4.511932**	**-1.467042**
C	**-0.252076**	**-3.758608**	**-1.213009**
C	**0.245324**	**-0.825684**	**-3.867754**
H	**3.158318**	**-0.985747**	**-4.651301**
H	**4.767839**	**-0.519974**	**-2.469641**
C	**0.251592**	**3.757888**	**1.218445**
H	**3.165877**	**4.517760**	**1.451708**
H	**4.771685**	**2.393668**	**0.761166**
C	**-0.245311**	**0.822753**	**3.869083**
H	**-3.158821**	**0.999710**	**4.649308**
H	**-4.768062**	**0.532520**	**2.467993**
C	**-0.252940**	**2.933602**	**-2.642599**
H	**-3.167536**	**3.517642**	**-3.180181**
H	**-4.772581**	**1.862561**	**-1.679753**
H	**-0.179171**	**1.812605**	**4.337649**
H	**-0.161960**	**0.078431**	**4.671002**
H	**0.610053**	**0.701885**	**3.200366**
H	**0.184696**	**4.657741**	**0.594240**
H	**-0.605304**	**3.119157**	**0.992480**
H	**0.172213**	**4.082087**	**2.263748**
H	**-0.194083**	**2.853409**	**-3.735186**
H	**-0.165546**	**3.997995**	**-2.390501**
H	**0.603955**	**2.409490**	**-2.213183**
H	**-0.149300**	**-4.606636**	**-0.524081**
H	**-0.207414**	**-4.161889**	**-2.232195**
H	**0.603884**	**-3.095635**	**-1.067485**
H	**0.171149**	**-0.099108**	**-4.686543**
H	**0.171114**	**-1.825362**	**-4.313948**
H	**-0.610573**	**-0.682848**	**-3.204164**
H	**0.171993**	**-2.798830**	**3.730344**
H	**-0.603128**	**-2.446328**	**2.173998**
H	**0.190696**	**-4.010432**	**2.445848**

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Cd	**0.000007**	**-0.000994**	**-0.018829**
C	**2.965869**	**3.520211**	**-0.131834**
C	**1.639324**	**3.046697**	**-0.021042**
N	**1.637687**	**1.698526**	**-0.019382**
N	**2.953531**	**1.286202**	**-0.137105**
C	**3.757746**	**2.386598**	**-0.198630**
N	**-1.637226**	**-1.698167**	**-0.063748**
N	**-2.953177**	**-1.283068**	**-0.169263**
C	**-3.757402**	**-2.381679**	**-0.257536**
C	**-2.965163**	**-3.516498**	**-0.221853**
C	**-1.638691**	**-3.045695**	**-0.099115**
B	**3.427748**	**-0.210638**	**-0.058681**
N	**2.837631**	**-1.062690**	**-1.237013**
N	**1.554793**	**-0.885311**	**-1.721427**
C	**1.350583**	**-1.845363**	**-2.648297**
C	**2.496161**	**-2.667434**	**-2.751482**
C	**3.400045**	**-2.150787**	**-1.836511**
B	**-3.427806**	**0.211243**	**-0.054544**
N	**-2.837802**	**1.092380**	**-1.211615**
N	**-1.553736**	**0.929529**	**-1.698096**
C	**-1.349316**	**1.913655**	**-2.599339**
C	**-2.495657**	**2.736929**	**-2.682706**
C	**-3.400928**	**2.194620**	**-1.784166**
N	**1.596153**	**-1.014318**	**1.510680**
N	**2.955569**	**-0.855913**	**1.282549**
C	**3.652137**	**-1.405411**	**2.316325**
C	**2.747029**	**-1.922060**	**3.230147**
C	**1.468882**	**-1.654597**	**2.691104**
N	**-1.597137**	**0.971916**	**1.537423**
N	**-2.956503**	**0.824039**	**1.301980**
C	**-3.654040**	**1.358613**	**2.342842**
C	**-2.749851**	**1.856316**	**3.267875**
C	**-1.471007**	**1.591917**	**2.728830**
N	**4.963292**	**-0.206528**	**-0.223728**
N	**-4.963317**	**0.210010**	**-0.218850**
C	**-0.377152**	**-3.859539**	**-0.020097**
H	**-4.830583**	**-2.287415**	**-0.324057**
H	**-3.297758**	**-4.545035**	**-0.268505**
H	**4.729341**	**-1.357818**	**2.324543**
H	**2.976867**	**-2.419518**	**4.163310**
C	**0.129678**	**-2.005339**	**3.278642**
C	**-0.132476**	**1.918380**	**3.331514**
H	**-2.980790**	**2.339777**	**4.208089**
H	**-4.731454**	**1.316126**	**2.346839**
C	**-0.070688**	**2.019036**	**-3.384430**
H	**-2.643902**	**3.603145**	**-3.314429**
H	**-4.399626**	**2.511017**	**-1.523358**
C	**0.073441**	**-1.927633**	**-3.438582**
H	**2.644723**	**-3.516498**	**-3.405983**
H	**4.397840**	**-2.475218**	**-1.582182**
C	**0.378500**	**3.858833**	**0.082049**
H	**3.298708**	**4.549515**	**-0.151804**
H	**4.830805**	**2.293845**	**-0.269139**
N	**5.834793**	**-0.055519**	**0.842799**
C	**7.042913**	**0.173966**	**0.311260**
C	**6.972888**	**0.202320**	**-1.108652**
C	**5.644135**	**-0.032732**	**-1.404746**
H	**5.137798**	**-0.073173**	**-2.357772**
H	**7.777116**	**0.366039**	**-1.814631**
C	**8.248552**	**0.349209**	**1.195517**
C	**-5.645101**	**0.063786**	**-1.403064**
C	**-6.973641**	**-0.178106**	**-1.111444**
C	**-7.042151**	**-0.184704**	**0.308828**
N	**-5.833546**	**0.032112**	**0.844554**
C	**-8.246746**	**-0.381831**	**1.189898**
H	**-7.778573**	**-0.324694**	**-1.820383**
H	**-5.139572**	**0.126901**	**-2.355274**
H	**-0.016560**	**1.429576**	**4.306705**
H	**0.690060**	**1.596085**	**2.689679**
H	**-0.035397**	**2.998527**	**3.498122**
H	**0.278788**	**3.056974**	**-3.424741**
H	**0.716883**	**1.402488**	**-2.944930**
H	**-0.225839**	**1.687875**	**-4.420231**
H	**-0.477035**	**-4.646210**	**0.737460**
H	**-0.168253**	**-4.355154**	**-0.976610**
H	**0.486458**	**-3.241695**	**0.236011**
H	**-0.275136**	**-2.964075**	**-3.511320**
H	**-0.715380**	**-1.325240**	**-2.981968**
H	**0.230126**	**-1.564766**	**-4.463502**
H	**0.052456**	**-1.639094**	**4.309329**
H	**-0.691216**	**-1.576288**	**2.700165**
H	**-0.008537**	**-3.093680**	**3.311304**
H	**0.469695**	**4.606826**	**0.879002**
H	**0.183567**	**4.401769**	**-0.851342**
H	**-0.489374**	**3.231435**	**0.296685**
H	**-7.940530**	**-0.445752**	**2.238507**
H	**-8.955434**	**0.450720**	**1.088470**
H	**-8.784652**	**-1.301666**	**0.928639**
H	**8.786074**	**1.275327**	**0.956601**
H	**7.943673**	**0.386948**	**2.245776**
H	**8.957171**	**-0.480481**	**1.072478**

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Cd	**0.000861**	**-0.000193**	**0.000076**
C	**0.007040**	**3.881447**	**2.538800**
C	**0.013573**	**3.250710**	**1.282119**
N	**0.003010**	**1.916926**	**1.446558**
N	**-0.012700**	**1.676428**	**2.799805**
C	**-0.011287**	**2.855995**	**3.477883**
N	**0.066814**	**-1.915843**	**-1.445751**
N	**0.069210**	**-1.675291**	**-2.799071**
C	**0.108978**	**-2.854277**	**-3.476941**
C	**0.132586**	**-3.879476**	**-2.537680**
C	**0.103439**	**-3.249142**	**-1.281117**
B	**-0.031983**	**0.238527**	**3.395541**
N	**1.243553**	**-0.544114**	**2.966951**
N	**1.543596**	**-0.807728**	**1.651764**
C	**2.700131**	**-1.492107**	**1.639468**
C	**3.155156**	**-1.673951**	**2.957387**
C	**2.209583**	**-1.062034**	**3.773029**
B	**0.030744**	**-0.237922**	**-3.395248**
N	**1.283145**	**0.569624**	**-2.945423**
N	**1.556532**	**0.837857**	**-1.625353**
C	**2.698956**	**1.544982**	**-1.593951**
C	**3.171157**	**1.737675**	**-2.904266**
C	**2.251366**	**1.107644**	**-3.735465**
N	**-1.590801**	**-0.778380**	**1.619948**
N	**-1.312952**	**-0.520251**	**2.941102**
C	**-2.303448**	**-1.022268**	**3.727330**
C	**-3.241858**	**-1.619186**	**2.892532**
C	**-2.757390**	**-1.444619**	**1.584096**
N	**-1.578809**	**0.745367**	**-1.646171**
N	**-1.272551**	**0.495235**	**-2.962562**
C	**-2.259106**	**0.978365**	**-3.765391**
C	**-3.224295**	**1.554062**	**-2.946392**
C	**-2.759425**	**1.387202**	**-1.629850**
H	**-0.043174**	**0.322058**	**4.590186**
H	**0.041213**	**-0.321450**	**-4.589913**
H	**0.107835**	**-3.687463**	**-0.292846**
H	**0.117884**	**-2.888351**	**-4.556131**
Br	**0.191226**	**-5.755849**	**-2.893065**
H	**-2.278563**	**-0.925682**	**4.802474**
Br	**-4.854949**	**-2.493918**	**3.424775**
H	**-3.188085**	**-1.761566**	**0.644477**
H	**-3.212941**	**1.693566**	**-0.697481**
Br	**-4.845623**	**2.395883**	**-3.505946**
H	**-2.213270**	**0.884328**	**-4.840057**
H	**3.122136**	**1.876387**	**-0.655939**
Br	**4.748832**	**2.671039**	**-3.443075**
H	**2.225142**	**1.010746**	**-4.810519**
H	**3.144578**	**-1.816124**	**0.708725**
Br	**4.741975**	**-2.575797**	**3.522334**
H	**2.164308**	**-0.964833**	**4.847424**
H	**0.026464**	**3.689137**	**0.293964**
Br	**0.018981**	**5.758680**	**2.894256**
H	**-0.022214**	**2.890142**	**4.557017**

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Cd	**0.000001**	**0.000716**	**0.000952**
C	**-2.808805**	**-3.730861**	**-0.022443**
C	**-1.516446**	**-3.157755**	**-0.024464**
N	**-1.579423**	**-1.815024**	**-0.017878**
N	**-2.910417**	**-1.485128**	**-0.011659**
C	**-3.657397**	**-2.624772**	**-0.014316**
N	**1.580843**	**1.814980**	**0.043805**
N	**2.911558**	**1.483955**	**0.039764**
C	**3.659462**	**2.622410**	**0.076452**
C	**2.811781**	**3.728835**	**0.105678**
C	**1.518944**	**3.157201**	**0.083750**
B	**-3.407216**	**-0.010565**	**-0.001099**
N	**-2.917316**	**0.738416**	**-1.273992**
N	**-1.587864**	**0.916780**	**-1.558743**
C	**-1.530834**	**1.594282**	**-2.718345**
C	**-2.825732**	**1.871855**	**-3.213240**
C	**-3.669350**	**1.306360**	**-2.258186**
B	**3.407246**	**0.009495**	**-0.000253**
N	**2.916833**	**-0.695058**	**-1.298072**
N	**1.587265**	**-0.862037**	**-1.589158**
C	**1.529823**	**-1.500035**	**-2.770925**
C	**2.824530**	**-1.762175**	**-3.274601**
C	**3.668507**	**-1.230212**	**-2.300758**
N	**-1.589419**	**0.886019**	**1.576649**
N	**-2.918569**	**0.720057**	**1.282993**
C	**-3.671796**	**1.285048**	**2.267980**
C	**-2.829335**	**1.836012**	**3.232534**
C	**-1.533851**	**1.552994**	**2.742408**
N	**1.588661**	**-0.938672**	**1.545963**
N	**2.917991**	**-0.764210**	**1.258101**
C	**3.670650**	**-1.363084**	**2.223308**
C	**2.827597**	**-1.945268**	**3.168825**
C	**1.532399**	**-1.644694**	**2.688462**
H	**-4.607120**	**-0.014676**	**-0.001693**
H	**4.607159**	**0.012731**	**-0.000662**
H	**0.553661**	**3.649255**	**0.094494**
H	**4.740339**	**2.569862**	**0.079035**
C	**3.190150**	**5.188562**	**0.149538**
H	**-4.752408**	**1.257899**	**2.217274**
C	**-3.214593**	**2.560367**	**4.498554**
H	**-0.570875**	**1.798496**	**3.174172**
H	**0.569149**	**-1.903558**	**3.111740**
C	**3.212150**	**-2.711934**	**4.409896**
H	**4.751320**	**-1.335308**	**2.173557**
H	**0.566185**	**-1.741310**	**-3.203497**
C	**3.207834**	**-2.452521**	**-4.560071**
H	**4.749174**	**-1.197699**	**-2.254619**
H	**-0.567347**	**1.850886**	**-3.142353**
C	**-3.209465**	**2.605070**	**-4.474611**
H	**-4.749991**	**1.270998**	**-2.213530**
H	**-0.550776**	**-3.649123**	**-0.030538**
C	**-3.186062**	**-5.191525**	**-0.028887**
H	**-4.738314**	**-2.573209**	**-0.010397**
H	**-4.298654**	**2.668799**	**-4.576208**
H	**-2.817266**	**3.630630**	**-4.484100**
H	**-2.824140**	**2.101506**	**-5.371225**
H	**-4.303832**	**2.630818**	**4.595045**
H	**-2.837447**	**2.046102**	**5.392507**
H	**-2.815376**	**3.583096**	**4.519372**
H	**-4.274688**	**-5.316236**	**-0.020916**
H	**-2.802109**	**-5.707005**	**-0.919209**
H	**-2.787903**	**-5.718242**	**0.848538**
H	**4.296961**	**-2.517191**	**-4.661751**
H	**2.811443**	**-3.475465**	**-4.606160**
H	**2.826428**	**-1.916332**	**-5.439293**
H	**4.278883**	**5.312193**	**0.160100**
H	**2.805166**	**5.734927**	**-0.721697**
H	**2.793758**	**5.684723**	**1.045387**
H	**4.301349**	**-2.786131**	**4.504220**
H	**2.835022**	**-2.227764**	**5.320536**
H	**2.812412**	**-3.734579**	**4.396288**

Model 10

91

Cd	**-0.000014**	**0.032082**	**0.000479**
N	**5.823544**	**0.306378**	**1.033751**
N	**4.982067**	**-0.128205**	**0.030650**
C	**5.675096**	**-0.940769**	**-0.839293**
C	**6.994882**	**-1.021646**	**-0.423325**
C	**7.020343**	**-0.218778**	**0.748936**
B	**3.448797**	**0.026800**	**0.081613**
N	**2.963883**	**1.281839**	**0.883592**
N	**1.615925**	**1.577005**	**0.883854**
C	**1.473540**	**2.709216**	**1.591462**
C	**2.718037**	**3.180875**	**2.061779**
C	**3.632201**	**2.242431**	**1.588287**
N	**-1.615850**	**1.576293**	**-0.884092**
N	**-2.963761**	**1.280926**	**-0.884106**
C	**-3.631960**	**2.240803**	**-1.589857**
C	**-2.717804**	**3.179101**	**-2.063630**
C	**-1.473387**	**2.707925**	**-1.592577**
B	**-3.448849**	**0.026506**	**-0.081325**
N	**-4.982147**	**-0.128461**	**-0.031169**
N	**-5.822989**	**0.306270**	**-1.034729**
C	**-7.020197**	**-0.218164**	**-0.750279**
C	**-6.995347**	**-1.021723**	**0.421520**
C	**-5.675721**	**-0.941297**	**0.838098**
N	**-1.643617**	**-0.057871**	**1.767961**
C	**-1.516291**	**0.371077**	**3.034874**
C	**-2.723539**	**0.922530**	**3.518373**
C	**-3.594022**	**0.803091**	**2.438834**
N	**-2.944588**	**0.195606**	**1.399028**
N	**1.643230**	**-0.058875**	**-1.767327**
N	**2.944251**	**0.194784**	**-1.398726**
C	**3.593816**	**0.801116**	**-2.439138**
C	**2.723212**	**0.919950**	**-3.518640**
C	**1.515687**	**0.369878**	**-3.034274**
N	**-1.527544**	**-1.498129**	**-0.926350**
N	**-2.870774**	**-1.277612**	**-0.742768**
C	**-3.570834**	**-2.302571**	**-1.318791**
C	**-2.677876**	**-3.213054**	**-1.875739**
C	**-1.410693**	**-2.653851**	**-1.597190**
N	**1.527763**	**-1.497273**	**0.928313**
N	**2.870925**	**-1.276910**	**0.744004**
C	**3.571179**	**-2.301538**	**1.320395**
C	**2.678442**	**-3.211702**	**1.878200**
C	**1.411161**	**-2.652492**	**1.600084**
H	**0.560518**	**0.270120**	**-3.536220**
H	**4.627633**	**1.102738**	**-2.349686**
C	**3.011949**	**1.491968**	**-4.884392**
H	**-4.701754**	**2.166491**	**-1.713812**
C	**-3.003642**	**4.410117**	**-2.888046**
H	**-0.484584**	**3.129055**	**-1.730608**
H	**0.484725**	**3.130396**	**1.729336**
C	**3.003931**	**4.412560**	**2.885165**
H	**4.702049**	**2.168371**	**1.711928**
H	**0.425420**	**-3.026977**	**1.849464**
C	**2.999046**	**-4.491796**	**2.609389**
H	**4.651737**	**-2.316152**	**1.308757**
H	**-0.424865**	**-3.028498**	**-1.845966**
C	**-2.998115**	**-4.493433**	**-2.606565**
H	**-4.651401**	**-2.317079**	**-1.307651**
H	**-0.561323**	**0.271073**	**3.537153**
C	**-3.012039**	**1.496284**	**4.883446**
H	**-4.627625**	**1.105298**	**2.348900**
H	**-5.183721**	**-1.412055**	**1.677649**
C	**-8.130273**	**-1.774822**	**1.070497**
H	**-7.862733**	**0.001330**	**-1.397358**
H	**7.863215**	**0.000304**	**1.395712**
C	**8.129363**	**-1.774633**	**-1.073209**
H	**5.182698**	**-1.410964**	**-1.678926**
H	**-4.080865**	**-4.628773**	**-2.704031**
H	**-2.572108**	**-4.499813**	**-3.618404**
H	**-2.601301**	**-5.372385**	**-2.081015**
H	**-2.459984**	**4.396119**	**-3.842021**
H	**-4.071836**	**4.486310**	**-3.118900**
H	**-2.713262**	**5.329269**	**-2.361727**
H	**-3.995730**	**1.977855**	**4.908541**
H	**-3.003879**	**0.721011**	**5.661515**
H	**-2.266864**	**2.249748**	**5.168787**
H	**4.081890**	**-4.627725**	**2.705289**
H	**2.574589**	**-4.497258**	**3.621889**
H	**2.600929**	**-5.370868**	**2.085031**
H	**2.266013**	**2.244034**	**-5.171448**
H	**3.995047**	**1.974757**	**-4.909489**
H	**3.005388**	**0.715487**	**-5.661285**
H	**2.713805**	**5.331314**	**2.357995**
H	**2.460079**	**4.399478**	**3.839040**
H	**4.072092**	**4.488772**	**3.116165**
H	**8.617605**	**-2.459195**	**-0.367130**
H	**7.773623**	**-2.372443**	**-1.919765**
H	**8.904397**	**-1.094725**	**-1.452343**
H	**-7.774934**	**-2.373858**	**1.916357**
H	**-8.904918**	**-1.094907**	**1.450397**
H	**-8.618895**	**-2.458249**	**0.363578**

Model 11

89			
Cd	-0.000007	0.000671	0.001874
C	2.837964	-2.534641	2.709192
C	1.532412	-2.166731	2.317042
N	1.598176	-1.246134	1.337339
N	2.938940	-1.009983	1.087136
C	3.703400	-1.787246	1.914786
N	-1.597681	1.246126	-1.336238
N	-2.938632	1.010282	-1.086373
C	-3.702625	1.781581	-1.920089
C	-2.836713	2.524708	-2.717988
C	-1.531388	2.160801	-2.321440
B	3.411465	0.004813	0.002124
N	2.935394	1.451068	0.337210
N	1.593755	1.783419	0.412586
C	1.524609	3.093144	0.714989
C	2.828794	3.620020	0.837531
C	3.696963	2.559216	0.593468
B	-3.411565	-0.003086	-0.000097
N	-2.937926	0.430970	1.420363
N	-1.596905	0.531470	1.748461
C	-1.530111	0.924643	3.033925
C	-2.835243	1.082007	3.549093
C	-3.701529	0.763023	2.506787
N	1.598075	-0.532402	-1.747017
N	2.938935	-0.429346	-1.418733
C	3.703317	-0.758794	-2.505389
C	2.837866	-1.078364	-3.548198
C	1.532347	-0.924108	-3.033088
N	-1.595580	-1.782736	-0.413453
N	-2.936918	-1.449852	-0.334914
C	-3.699608	-2.557032	-0.591957
C	-2.832450	-3.617932	-0.839342
C	-1.527744	-3.092039	-0.718065
H	4.604468	0.006601	0.002565
H	-4.604569	-0.003897	0.000125
C	-0.222929	2.669384	-2.859738
C	-5.207314	1.785779	-1.929825
H	-3.116683	3.235679	-3.485542
C	5.207969	-0.759541	-2.515101
H	3.118298	-1.383154	-4.548923
C	0.224280	-1.141165	-3.741794
C	-0.218427	-3.811838	-0.885535
H	-3.111249	-4.637265	-1.076367
C	-5.204290	-2.568507	-0.594143
C	-0.221520	1.140283	3.742141
H	-3.114875	1.387867	4.549705
C	-5.206198	0.765064	2.517179
C	0.214642	3.811645	0.883054
H	3.106641	4.640157	1.072390
C	5.201591	2.572201	0.596435
C	0.224284	-2.672265	2.859011
H	3.118440	-3.251218	3.471366
C	5.208064	-1.792835	1.922036
H	0.113038	4.206443	1.902068
H	0.147520	4.665465	0.197110
H	-0.630673	3.147775	0.688458
H	-0.134841	0.477880	4.612853
H	0.625475	0.947329	3.079950
H	-0.142305	2.170891	4.110712
H	0.159380	-3.763637	2.765652
H	0.123599	-2.432115	3.925221
H	-0.622727	-2.231427	2.328576
H	0.150886	-2.168994	-4.119148
H	-0.623015	-0.958887	-3.077012
H	0.132603	-0.471589	-4.606490
H	-0.141247	-4.253387	-1.887196
H	0.627777	-3.136018	-0.742930
H	-0.128355	-4.632331	-0.162303
H	-0.126934	3.750511	-2.696839
H	0.623915	2.175200	-2.378308
H	-0.153022	2.497656	-3.941271
H	-5.562436	2.488987	-2.689591
H	-5.620333	0.797389	-2.164395
H	-5.624191	2.093230	-0.963269
H	-5.560913	1.068378	3.507144
H	-5.622111	1.462740	1.780436
H	-5.620530	-0.226461	2.298684
H	5.563846	-2.500623	2.677212
H	5.623383	-2.094892	0.953101
H	5.621933	-0.806061	2.161733
H	5.563382	-1.061331	-3.505286
H	5.621632	0.231936	-2.294988
H	5.623821	-1.458004	-1.779119
H	-5.558238	-3.577455	-0.827718
H	-5.619641	-2.281302	0.379274
H	-5.620009	-1.882702	-1.342070
H	5.554379	3.581582	0.830045
H	5.617718	1.886887	1.344567
H	5.617491	2.285363	-0.376825

Model 12

53

Cd	**0.000009**	**-0.000286**	**0.000461**
N	**-1.583978**	**0.841811**	**1.603301**
N	**-1.578817**	**-1.812594**	**-0.070051**
N	**1.583508**	**-0.946005**	**-1.543872**
N	**-1.583465**	**0.963282**	**-1.532919**
N	**1.584368**	**-0.860642**	**1.593280**
N	**1.578407**	**1.813046**	**-0.049182**
N	**-2.911736**	**-1.480112**	**-0.059280**
N	**-2.915954**	**0.682160**	**1.307046**
N	**-2.915568**	**0.784107**	**-1.248700**
B	**-3.406365**	**-0.005466**	**-0.000383**
H	**-4.606242**	**-0.007606**	**-0.000584**
N	**2.916276**	**-0.697091**	**1.298811**
N	**2.915599**	**-0.769395**	**-1.257974**
N	**2.911419**	**1.480842**	**-0.042290**
B	**3.406387**	**0.005689**	**-0.000621**
H	**4.606250**	**0.008127**	**-0.001018**
C	**1.515734**	**3.154848**	**-0.087023**
C	**3.663145**	**2.614585**	**-0.075359**
C	**2.808999**	**3.712866**	**-0.105422**
H	**0.553221**	**3.649270**	**-0.098413**
H	**4.742710**	**2.559211**	**-0.074787**
H	**3.082449**	**4.758494**	**-0.134758**
C	**-1.525672**	**1.466486**	**2.791609**
C	**-3.671376**	**1.206666**	**2.309951**
C	**-2.820737**	**1.720956**	**3.283890**
H	**-4.750746**	**1.176883**	**2.259135**
H	**-3.097499**	**2.206755**	**4.209275**
H	**-0.564786**	**1.700685**	**3.230753**
C	**1.526367**	**-1.498532**	**2.774563**
C	**3.671942**	**-1.232400**	**2.295808**
C	**2.821556**	**-1.758380**	**3.263711**
H	**0.565590**	**-1.738233**	**3.210971**
H	**3.098572**	**-2.254880**	**4.183331**
H	**4.751288**	**-1.201697**	**2.245254**
C	**1.524692**	**-1.649056**	**-2.687515**
C	**3.670590**	**-1.361943**	**-2.222571**
C	**2.819547**	**-1.937765**	**-3.161069**
H	**0.563609**	**-1.909354**	**-3.111264**
H	**3.095933**	**-2.483524**	**-4.052512**
H	**4.749972**	**-1.330487**	**-2.173345**
C	**-1.524602**	**1.679914**	**-2.668110**
C	**-3.670523**	**1.388760**	**-2.205789**
C	**-2.819435**	**1.975505**	**-3.137457**
H	**-0.563511**	**1.944521**	**-3.089157**
H	**-3.095780**	**2.532272**	**-4.022086**
H	**-4.749915**	**1.357417**	**-2.156548**
C	**-1.516536**	**-3.153862**	**-0.124170**
C	**-3.663783**	**-2.613171**	**-0.106010**
C	**-2.809953**	**-3.711281**	**-0.148679**
H	**-0.554170**	**-3.648382**	**-0.141979**
H	**-3.083706**	**-4.756415**	**-0.190534**
H	**-4.743323**	**-2.557497**	**-0.105151**

Model 13

67

Cd	**-0.000361**	**0.000054**	**-0.027239**
C	**2.594083**	**3.688532**	**0.337751**
C	**1.408629**	**3.099150**	**-0.139753**
N	**1.581175**	**1.785422**	**-0.360041**
N	**2.891203**	**1.501902**	**-0.038327**
C	**3.504076**	**2.640776**	**0.402027**
N	**-1.580804**	**-1.818870**	**0.049479**
N	**-2.889154**	**-1.469156**	**0.306414**
C	**-3.496094**	**-2.474025**	**1.005254**
C	**-2.584257**	**-3.507458**	**1.179992**
C	**-1.403823**	**-3.044957**	**0.568870**
B	**3.442880**	**0.028503**	**0.016533**
N	**2.906178**	**-0.832260**	**-1.186885**
N	**1.569476**	**-1.084389**	**-1.396392**
C	**1.488329**	**-1.910340**	**-2.449707**
C	**2.771566**	**-2.218340**	**-2.939102**
C	**3.641122**	**-1.520498**	**-2.110764**
B	**-3.443324**	**-0.023572**	**0.023594**
N	**-2.906543**	**0.540588**	**-1.344167**
N	**-1.570511**	**0.748510**	**-1.601182**
C	**-1.489208**	**1.307620**	**-2.817356**
C	**-2.771726**	**1.481737**	**-3.370324**
C	**-3.640996**	**0.987962**	**-2.406008**
N	**1.607815**	**-0.605411**	**1.640171**
N	**2.963240**	**-0.599260**	**1.367668**
C	**3.639169**	**-1.125355**	**2.429754**
C	**2.716431**	**-1.483275**	**3.406274**
C	**1.465442**	**-1.140488**	**2.862462**
N	**-1.611996**	**0.960362**	**1.466420**
N	**-2.966351**	**0.896738**	**1.196089**
C	**-3.643949**	**1.658123**	**2.103151**
C	**-2.723295**	**2.228739**	**2.974911**
C	**-1.471842**	**1.764166**	**2.531684**
N	**4.977130**	**0.102591**	**-0.126658**
N	**-4.977282**	**-0.131530**	**-0.098991**
H	**-0.438898**	**-3.528035**	**0.483898**
H	**-4.524591**	**-2.391147**	**1.323058**
H	**-2.754069**	**-4.454016**	**1.674228**
H	**4.713177**	**-1.216499**	**2.389931**
H	**2.924996**	**-1.928771**	**4.369066**
H	**0.475854**	**-1.251914**	**3.286217**
H	**-0.483417**	**1.967274**	**2.922841**
H	**-2.933466**	**2.886185**	**3.807128**
H	**-4.717315**	**1.741980**	**2.037767**
H	**-0.519562**	**1.552538**	**-3.230825**
H	**-3.032970**	**1.907781**	**-4.328935**
H	**-4.719500**	**0.936591**	**-2.403641**
H	**0.518297**	**-2.237715**	**-2.800477**
H	**3.033059**	**-2.857884**	**-3.770560**
H	**4.720004**	**-1.478241**	**-2.113852**
H	**0.443503**	**3.551413**	**-0.328554**
H	**2.768441**	**4.723918**	**0.595857**
H	**4.535018**	**2.632186**	**0.722435**
N	**5.837843**	**-0.796735**	**0.473139**
C	**7.039137**	**-0.554851**	**-0.062888**
C	**6.987092**	**0.478999**	**-1.028735**
C	**5.658474**	**0.865028**	**-1.046364**
H	**5.152790**	**1.607482**	**-1.646043**
H	**7.794665**	**0.887443**	**-1.621183**
H	**7.895382**	**-1.130166**	**0.267735**
C	**-5.657692**	**-1.090944**	**-0.811675**
C	**-6.986115**	**-0.711495**	**-0.888401**
C	**-7.038892**	**0.522693**	**-0.196678**
N	**-5.838167**	**0.885216**	**0.267842**
H	**-7.895228**	**1.160528**	**-0.014170**
H	**-7.793137**	**-1.249186**	**-1.367591**
H	**-5.151719**	**-1.955276**	**-1.215988**

Model 14

39

Cd	**-0.007735**	**-0.917485**	**0.040310**
C	**-2.888044**	**-0.912998**	**0.912895**
S	**-2.348960**	**-1.997699**	**-0.355439**
S	**2.322672**	**-2.012235**	**0.459539**
C	**2.871984**	**-0.961675**	**-0.832948**
N	**4.162881**	**-0.988533**	**-1.232913**
N	**-4.179533**	**-0.917523**	**1.311919**
S	**-1.732741**	**0.173767**	**1.662206**
S	**1.727724**	**0.120899**	**-1.604920**
C	**4.690986**	**-0.160041**	**-2.346854**
C	**5.924854**	**0.651746**	**-1.902338**
H	**4.964142**	**-0.843209**	**-3.167096**
H	**3.893184**	**0.493412**	**-2.700501**
C	**7.014415**	**-0.258005**	**-1.296816**
H	**6.312717**	**1.196893**	**-2.773702**
H	**5.608789**	**1.402170**	**-1.163813**
C	**6.422434**	**-1.138740**	**-0.176443**
H	**7.431740**	**-0.903091**	**-2.086120**
H	**7.845006**	**0.346286**	**-0.909348**
C	**5.177325**	**-1.909959**	**-0.659820**
H	**7.164058**	**-1.867048**	**0.179169**
H	**6.141693**	**-0.514465**	**0.683737**
H	**5.459168**	**-2.624666**	**-1.449685**
H	**4.716296**	**-2.468632**	**0.154945**
C	**-4.700064**	**-0.059466**	**2.406957**
C	**-5.925810**	**0.754253**	**1.943836**
H	**-4.980134**	**-0.721604**	**3.241997**
H	**-3.896081**	**0.593871**	**2.746517**
C	**-7.023851**	**-0.158211**	**1.358006**
H	**-6.308735**	**1.322657**	**2.802495**
H	**-5.602192**	**1.484921**	**1.188954**
C	**-6.439984**	**-1.068911**	**0.257527**
H	**-7.447486**	**-0.781805**	**2.161106**
H	**-7.848557**	**0.445254**	**0.956947**
C	**-5.202570**	**-1.841366**	**0.758345**
H	**-7.188415**	**-1.797684**	**-0.082531**
H	**-6.152909**	**-0.466315**	**-0.615924**
H	**-5.491589**	**-2.536109**	**1.563290**
H	**-4.746622**	**-2.421951**	**-0.043866**

(For models 15 and 16 contributions of several configurational isomers has been teaken into account. The corresponding averaged weights are also given together the relevant coordinates. Models contributing up to 1% have been neglected)

Model 15A avgd weight 33%

45

Cd	-0.008028	-0.863676	0.036512
C	5.216813	-1.716167	-0.399299
N	4.228304	-0.778082	-0.997344
C	4.772726	0.144166	-2.050542
C	6.033604	0.872023	-1.515377
C	7.093325	-0.079737	-0.923332
C	6.449434	-0.975861	0.152223
C	2.910696	-0.827088	-0.697323
S	2.310966	-1.945307	0.516601
S	-2.337936	-1.932884	-0.417884
C	-2.925767	-0.781538	0.770681
S	-1.777222	0.279644	1.567502
H	4.712684	-2.277946	0.387710
N	-4.242394	-0.712604	1.071122
C	-5.241585	-1.653991	0.496360
C	-6.467976	-0.913921	-0.069189
C	-7.100476	0.012631	0.987183
C	-6.029958	0.966854	1.555342
C	-4.775256	0.238610	2.104259
H	-4.744904	-2.238363	-0.278814
S	1.772793	0.225784	-1.520084
C	4.989825	-0.601395	-3.385716
H	3.996715	0.895108	-2.212895
H	6.457403	1.467773	-2.335371
H	5.715069	1.580422	-0.736926
H	7.529524	-0.707033	-1.715051
H	7.919454	0.502294	-0.493893
H	7.163910	-1.724688	0.520914
H	6.144624	-0.365491	1.014715
H	5.522730	-2.432268	-1.177206
C	-4.996793	-0.474438	3.456364
H	-3.991383	0.985169	2.248067
H	-6.445894	1.585235	2.362494
H	-5.706103	1.654192	0.760389
H	-7.541106	-0.592235	1.793767
H	-7.921737	0.593072	0.546405
H	-7.190747	-1.663614	-0.419471
H	-6.159014	-0.326197	-0.945821
H	-5.552920	-2.349341	1.290777
H	-5.302305	0.262976	4.209795
H	-5.774131	-1.246223	3.406640
H	-4.064858	-0.940789	3.795977
H	5.304280	0.115760	-4.154862
H	5.759274	-1.379606	-3.316840
H	4.053946	-1.065931	-3.716839

Model 15B avgd weight 35%

45

Cd	0.037175	-0.746877	0.055848
C	-4.808674	0.423402	1.886994
N	-4.222837	-0.590888	0.968935
C	-5.184879	-1.621964	0.452477
C	-6.432110	-0.927263	-0.152835
C	-7.083068	0.106488	0.789363
C	-6.027240	1.125781	1.259628
C	-2.897508	-0.650528	0.706953
S	-1.797646	0.538010	1.384646
S	1.811295	0.057379	-1.669533
C	2.953509	-0.831058	-0.676277
S	2.366584	-1.686048	0.740340
H	-4.026989	1.142248	2.134803
S	-2.252648	-1.923023	-0.316387
N	4.266293	-0.857600	-1.000971
C	5.257328	-1.663520	-0.236776
C	6.522140	-0.851517	0.097560
C	7.145293	-0.233516	-1.168837
C	6.084101	0.592685	-1.924203
C	4.791359	-0.200611	-2.245566
H	4.769802	-2.019065	0.671628
H	-4.660191	-2.134077	-0.356915
C	4.946902	-1.226967	-3.389924
H	4.024040	0.516403	-2.545248
H	6.490023	0.979609	-2.868895
H	5.808918	1.464454	-1.313075
H	7.540382	-1.031840	-1.814623
H	7.997273	0.406576	-0.904130
H	7.234710	-1.518564	0.601910
H	6.259923	-0.056765	0.811007
H	5.521949	-2.545175	-0.840415
H	-5.102561	-0.085013	2.817824
H	-6.449179	1.813717	2.005160
H	-5.690435	1.735319	0.408532
H	-7.526523	-0.396242	1.661754
H	-7.904863	0.617644	0.270594
H	-7.153406	-1.706335	-0.435333
H	-6.126475	-0.422342	-1.080628
C	-5.508962	-2.671733	1.538648
H	5.245914	-0.704861	-4.307930
H	5.704840	-1.989562	-3.174289
H	3.991884	-1.729733	-3.580804
H	-6.139883	-3.458745	1.105857
H	-4.586280	-3.137942	1.902908
H	-6.044392	-2.244484	2.394931

Model 15C avgd weight 32%

45

Cd	0.036302	-0.586123	-0.073602
C	-4.708422	0.165335	2.191762
N	-4.182733	-0.619287	1.041398
C	-5.173203	-1.534817	0.379666
C	-6.465845	-0.752897	0.028917
C	-7.055069	0.033949	1.217472
C	-5.976612	0.955139	1.819203
C	-2.874027	-0.611439	0.699594
S	-1.738800	0.438236	1.532033
S	1.824222	0.385997	-1.697379
C	2.946006	-0.662751	-0.845721
S	2.343190	-1.676884	0.453451
H	-3.917010	0.834111	2.531412
S	-2.284300	-1.657181	-0.580444
N	4.254297	-0.694605	-1.187615
C	5.231962	-1.612059	-0.509780
C	6.535836	-0.842411	-0.173731
C	7.135531	-0.085704	-1.376542
C	6.070003	0.839890	-1.994343
C	4.790391	0.061746	-2.352047
H	4.761064	-1.899302	0.432554
H	-4.706182	-1.845751	-0.557051
H	4.998141	-0.656728	-3.159861
H	4.008392	0.735565	-2.703344
H	6.446399	1.320430	-2.907737
H	5.815754	1.642556	-1.286862
H	7.494143	-0.796394	-2.136113
H	8.009577	0.495567	-1.054529
H	7.258878	-1.560044	0.237276
H	6.311855	-0.121453	0.625863
C	5.451040	-2.899436	-1.334979
H	-4.926745	-0.535471	3.012213
H	-6.346452	1.457376	2.723543
H	-5.710579	1.741231	1.097588
H	-7.424210	-0.657653	1.989516
H	-7.920506	0.621846	0.884417
H	-7.198934	-1.467421	-0.369523
H	-6.231253	-0.049803	-0.783450
C	-5.410891	-2.803850	1.227820
H	6.101057	-3.583959	-0.774891
H	4.494464	-3.405541	-1.508344
H	5.923225	-2.706091	-2.305611
H	-6.070535	-3.488941	0.679824
H	-4.461687	-3.320404	1.410657
H	-5.880434	-2.586417	2.194642

Model 16A avgd weight 33%

45

Cd	3.605132	-4.210370	1.944666
C	5.942225	-8.712768	3.555013
N	5.771692	-7.332973	4.074201
C	6.438355	-7.119010	5.382075
C	5.922589	-8.105569	6.457078
C	6.068705	-9.561334	5.957828
C	5.421985	-9.749639	4.570017
C	5.102262	-6.363485	3.411271
S	4.367562	-6.699790	1.854382
S	3.810799	-2.267057	0.222690
C	2.093086	-2.050773	0.503485
S	1.264234	-3.113177	1.626301
H	4.329993	-9.653147	4.647590
S	4.964680	-4.755505	4.097921
N	1.413761	-1.076295	-0.141611
C	2.039211	-0.153586	-1.120374
C	1.834164	1.328362	-0.724302
C	0.330267	1.622560	-0.520231
C	-0.314406	0.616301	0.455141
C	-0.041096	-0.840221	0.031443
H	0.079258	0.770467	1.469565
H	2.348693	1.480052	0.237406
H	-1.401490	0.766320	0.503333
C	2.476806	2.258252	-1.772034
H	5.419531	-8.792719	2.601715
H	3.100307	-0.395361	-1.194984
H	7.521074	-7.265648	5.232404
H	6.275169	-6.085276	5.689554
C	6.648090	-7.868556	7.796067
H	4.851053	-7.896076	6.600406
H	7.140709	-9.813884	5.899967
H	5.620279	-10.254168	6.683148
H	5.631325	-10.754496	4.178838
H	7.017392	-8.868049	3.372136
H	-0.528847	-1.052072	-0.933315
H	-0.422833	-1.546930	0.768447
H	-0.181059	1.566324	-1.495776
H	0.194758	2.648804	-0.151915
H	1.574064	-0.343419	-2.102133
H	6.266896	-8.547247	8.569063
H	7.728368	-8.045797	7.698807
H	6.505412	-6.840347	8.151883
H	2.357521	3.309612	-1.482430
H	3.550614	2.059079	-1.878854
H	2.009073	2.127998	-2.758006

Model 16B avgd weight 31%

45

Cd	3.623323	-4.203872	1.973446
C	2.030110	-0.185634	-1.133098
N	1.417738	-1.088577	-0.127129
C	-0.027875	-0.828902	0.080861
C	-0.287566	0.631564	0.522969
C	0.340359	1.614485	-0.491506
C	1.827608	1.291578	-0.743088
C	2.101157	-2.061756	0.515627
S	1.282318	-3.111862	1.657356
S	4.940878	-4.741438	4.151853
C	5.128031	-6.340997	3.456481
S	4.447398	-6.676287	1.875314
H	2.416889	1.504013	0.159946
S	3.814337	-2.287481	0.215522
N	5.792935	-7.304397	4.132525
C	6.387162	-7.100060	5.476236
C	5.840071	-8.120542	6.503498
C	6.051492	-9.561890	5.986359
C	5.483117	-9.739628	4.563388
C	6.025892	-8.668704	3.597074
H	4.386241	-9.674445	4.585280
H	5.740869	-10.730255	4.164778
H	2.229606	1.921895	-1.547958
C	-1.796739	0.874407	0.718616
H	0.215083	0.769454	1.493032
H	5.555056	-8.742442	2.616611
H	3.088367	-0.431713	-1.222535
H	7.479484	-7.217383	5.380879
H	6.182071	-6.077095	5.794403
C	6.484294	-7.892062	7.884695
H	4.757115	-7.941178	6.591378
H	7.131549	-9.785161	5.980562
H	5.584695	-10.280322	6.674293
H	7.112910	-8.791872	3.467142
H	-0.544345	-1.026140	-0.873308
H	-0.404038	-1.534538	0.822697
H	-0.214918	1.550623	-1.442296
H	0.231516	2.646892	-0.131513
H	1.545769	-0.391732	-2.100885
H	6.080641	-8.597233	8.621886
H	7.572911	-8.037648	7.844108
H	6.292924	-6.875922	8.252289
H	-1.983299	1.901462	1.056296
H	-2.347873	0.726067	-0.220623
H	-2.217766	0.192715	1.468531

Model 16c avgd weight 31%

45

Cd	3.685653	-4.126219	1.971125
C	2.008096	-0.151566	-1.143588
N	1.404262	-1.097970	-0.173820
C	-0.057103	-0.900652	-0.005574
C	-0.370805	0.543603	0.431437
C	0.253758	1.575866	-0.529820
C	1.765228	1.320613	-0.730662
C	2.109604	-2.049669	0.477689
S	3.828289	-2.234980	0.183147
S	4.485820	-6.602088	2.028662
C	5.273991	-6.146145	3.528379
S	5.140508	-4.494583	4.102405
C	2.389747	2.279678	-1.762894
N	5.978724	-7.059158	4.233719
C	6.125220	-8.477212	3.823268
C	5.628331	-9.444508	4.925166
C	6.347697	-9.146163	6.260659
C	6.238576	-7.654925	6.640060
C	6.703542	-6.741418	5.489264
S	1.313586	-3.112831	1.624220
H	4.552903	-9.251722	5.062708
H	2.271697	1.472438	0.235298
C	5.806383	-10.908412	4.477367
H	6.848668	-7.435557	7.526809
H	3.075033	-0.365305	-1.219219
H	5.574852	-8.628067	2.893694
H	-0.533108	-1.114582	-0.975657
H	-0.425020	-1.624733	0.721452
H	-1.461660	0.665335	0.474471
H	0.012805	0.696974	1.449803
H	-0.251846	1.518387	-1.508296
H	0.091781	2.594296	-0.150691
H	1.549111	-0.342499	-2.127846
H	7.777867	-6.891386	5.297217
H	6.543359	-5.689639	5.726752
H	7.410879	-9.422940	6.163965
H	5.930244	-9.773155	7.060559
H	7.194125	-8.659479	3.622709
H	2.242634	3.323831	-1.460167
H	3.468769	2.108988	-1.866298
H	1.930493	2.150959	-2.753012
H	5.198458	-7.405737	6.892581
H	5.430113	-11.596637	5.244357
H	5.260858	-11.111661	3.547183
H	6.865924	-11.145229	4.306729

Model 17

63

Cd	**-0.002040**	**0.002283**	**-0.227365**
C	**1.633343**	**1.684390**	**2.229040**
C	**3.703429**	**1.682518**	**1.369738**
C	**2.969117**	**2.028038**	**2.508116**
C	**3.704370**	**-1.822977**	**-1.539627**
C	**2.969412**	**-3.007487**	**-1.657107**
C	**1.631448**	**-2.666889**	**-1.391265**
C	**5.181910**	**-1.616065**	**-1.727169**
C	**0.409992**	**-3.542985**	**-1.413956**
C	**5.178225**	**1.845425**	**1.124832**
C	**0.414871**	**1.861380**	**3.092081**
C	**-1.620039**	**2.660742**	**-1.427715**
C	**-2.956026**	**3.008080**	**-1.691813**
C	**-3.701413**	**1.832900**	**-1.545045**
C	**-5.181536**	**1.635925**	**-1.722503**
C	**-0.397435**	**3.535638**	**-1.429653**
C	**-3.706802**	**-1.680258**	**1.375325**
C	**-2.966559**	**-2.039993**	**2.505668**
C	**-1.631003**	**-1.701464**	**2.220625**
C	**-0.406754**	**-1.898645**	**3.070876**
C	**-5.183955**	**-1.833697**	**1.138773**
N	**1.563355**	**1.161100**	**0.986430**
N	**2.841462**	**1.155661**	**0.456752**
N	**1.560661**	**-1.342646**	**-1.134276**
N	**2.839941**	**-0.822728**	**-1.218564**
N	**-1.558985**	**1.340628**	**-1.147407**
N	**-2.843771**	**0.830846**	**-1.212653**
N	**-1.566458**	**-1.167146**	**0.981913**
N	**-2.848396**	**-1.150897**	**0.460839**
B	**3.069546**	**0.718649**	**-1.037406**
B	**-3.083438**	**-0.709629**	**-1.031504**
H	**2.247186**	**1.293293**	**-1.717675**
H	**4.194250**	**0.990452**	**-1.356848**
H	**3.355234**	**2.478831**	**3.413664**
H	**-0.482005**	**1.473470**	**2.599926**
H	**0.529392**	**1.341601**	**4.051243**
H	**0.244229**	**2.922117**	**3.315010**
H	**5.376438**	**2.503144**	**0.270708**
H	**5.651495**	**2.278986**	**2.011287**
H	**5.662845**	**0.884567**	**0.914817**
H	**3.355916**	**-3.986122**	**-1.911717**
H	**-0.311621**	**-3.247245**	**-0.645554**
H	**-0.101669**	**-3.483421**	**-2.383406**
H	**0.687423**	**-4.588517**	**-1.245204**
H	**5.390740**	**-0.889563**	**-2.520728**
H	**5.659273**	**-1.245543**	**-0.811939**
H	**5.653997**	**-2.566066**	**-1.996000**
H	**-3.334090**	**3.984545**	**-1.966454**
H	**-0.621265**	**4.495499**	**-1.905057**
H	**-0.046227**	**3.737482**	**-0.409649**
H	**0.431073**	**3.065656**	**-1.970877**
H	**-5.656523**	**1.278453**	**-0.800891**
H	**-5.647392**	**2.587078**	**-1.997955**
H	**-5.400728**	**0.903246**	**-2.507558**
H	**-3.348836**	**-2.497560**	**3.409440**
H	**-2.271260**	**-1.290186**	**-1.717864**
H	**-4.213388**	**-0.971097**	**-1.340971**
H	**-0.515884**	**-1.403656**	**4.043573**
H	**-0.233749**	**-2.964661**	**3.265240**
H	**0.486702**	**-1.497893**	**2.582847**
H	**-5.653438**	**-2.273539**	**2.024124**
H	**-5.665249**	**-0.868612**	**0.940905**
H	**-5.390611**	**-2.482247**	**0.279685**

Model 18

63

Cd	**0.321754**	**0.102304**	**-0.013942**
S	**2.571285**	**-1.330405**	**0.721611**
S	**2.525518**	**1.325632**	**-0.712095**
B	**-2.991967**	**-0.122364**	**0.042549**
N	**-1.073382**	**-1.392391**	**-1.119508**
N	**-2.428797**	**-1.247822**	**-0.885364**
N	**-1.342813**	**1.702322**	**-0.690960**
N	**-2.651809**	**1.287628**	**-0.528090**
N	**-1.115860**	**-0.136707**	**1.812790**
N	**-2.458536**	**-0.269997**	**1.504082**
N	**4.782672**	**0.005544**	**-0.057944**
C	**-0.912896**	**-2.430819**	**-1.958874**
C	**-2.175304**	**-2.972586**	**-2.276056**
C	**-3.111179**	**-2.205027**	**-1.584468**
C	**0.443977**	**-2.851043**	**-2.451417**
C	**-4.607640**	**-2.356744**	**-1.569068**
C	**-1.379095**	**2.949680**	**-1.193256**
C	**-2.720121**	**3.353153**	**-1.358507**
C	**-3.501580**	**2.281514**	**-0.928769**
C	**-0.126319**	**3.721444**	**-1.509250**
C	**-5.001926**	**2.180103**	**-0.887806**
C	**-0.988021**	**-0.291774**	**3.142903**
C	**-2.256853**	**-0.531755**	**3.709181**
C	**-3.163498**	**-0.511788**	**2.651014**
C	**0.340816**	**-0.171543**	**3.835751**
C	**-4.652772**	**-0.717871**	**2.700240**
C	**5.550011**	**1.093828**	**-0.713667**
C	**5.954895**	**2.222186**	**0.252136**
C	**5.603685**	**-1.070344**	**0.551509**
C	**5.963101**	**-2.194669**	**-0.436294**
C	**3.426897**	**-0.008863**	**-0.014589**
H	**-4.178697**	**-0.235890**	**0.073151**
H	**-2.383309**	**-3.815890**	**-2.922257**
H	**1.222706**	**-2.611537**	**-1.719502**
H	**0.466884**	**-3.929556**	**-2.641725**
H	**0.697224**	**-2.342789**	**-3.391723**
H	**-4.990531**	**-2.552916**	**-0.560473**
H	**-5.114694**	**-1.459676**	**-1.943871**
H	**-4.892948**	**-3.197842**	**-2.208323**
H	**-3.077234**	**4.301474**	**-1.739932**
H	**0.448028**	**3.243074**	**-2.312404**
H	**-0.379075**	**4.735930**	**-1.832841**
H	**0.531887**	**3.795810**	**-0.635765**
H	**-5.438521**	**3.110069**	**-1.264791**
H	**-5.375712**	**1.356029**	**-1.507337**
H	**-5.375346**	**2.020432**	**0.130913**
H	**-2.487313**	**-0.700236**	**4.753487**
H	**1.164401**	**-0.441193**	**3.166540**
H	**0.511133**	**0.856479**	**4.183706**
H	**0.377804**	**-0.827085**	**4.712738**
H	**-5.201152**	**0.155807**	**2.328414**
H	**-4.967394**	**-1.581695**	**2.102506**
H	**-4.959775**	**-0.894161**	**3.735703**
H	**4.940564**	**1.494570**	**-1.527336**
H	**6.442316**	**0.634185**	**-1.156285**
H	**6.541755**	**2.976131**	**-0.288654**
H	**5.066299**	**2.709096**	**0.668153**
H	**6.569543**	**1.844702**	**1.078791**
H	**5.047027**	**-1.477998**	**1.398600**
H	**6.514949**	**-0.597477**	**0.938063**
H	**6.593818**	**-2.938884**	**0.067285**
H	**5.056438**	**-2.694988**	**-0.792996**
H	**6.518393**	**-1.810729**	**-1.301183**

Model 19

75

Cd	**0.310681**	**0.014856**	**-0.196569**
C	**1.679554**	**-0.574908**	**3.571620**
C	**2.455032**	**-1.597100**	**2.994660**
C	**2.636752**	**-2.791061**	**3.721989**
C	**2.056396**	**-2.958360**	**4.981751**
C	**1.279608**	**-1.935832**	**5.540622**
C	**1.093276**	**-0.745550**	**4.828636**
C	**3.116189**	**-1.425556**	**1.686538**
C	**4.605891**	**-1.441943**	**0.033639**
C	**4.409302**	**-1.883557**	**1.330079**
C	**-2.513057**	**0.608158**	**0.790460**
C	**-4.021801**	**0.835256**	**2.754888**
C	**-4.587184**	**-0.531518**	**3.187000**
C	**0.334108**	**-2.213908**	**-2.861578**
C	**1.166019**	**-2.408136**	**-3.991246**
C	**2.315376**	**-1.679663**	**-3.729381**
C	**-0.976556**	**-2.834589**	**-2.597697**
C	**-1.850219**	**-3.119762**	**-3.665554**
C	**-3.075945**	**-3.749907**	**-3.438325**
C	**-3.453675**	**-4.106502**	**-2.137887**
C	**-2.593990**	**-3.827781**	**-1.069060**
C	**-1.366135**	**-3.201547**	**-1.295747**
C	**3.389509**	**2.332999**	**-2.371681**
C	**2.673649**	**3.486566**	**-2.097583**
C	**1.620500**	**3.079349**	**-1.242759**
C	**0.598532**	**3.940120**	**-0.617926**
C	**0.132598**	**3.704826**	**0.688598**
C	**-0.810941**	**4.553328**	**1.273210**
C	**-1.303837**	**5.656713**	**0.567295**
C	**-0.844814**	**5.904638**	**-0.732221**
C	**0.096964**	**5.055469**	**-1.318056**
C	**-4.794594**	**1.509050**	**0.438007**
C	**-5.697742**	**0.451372**	**-0.224120**
N	**2.562169**	**-0.752595**	**0.648900**
N	**3.494832**	**-0.765396**	**-0.365270**
N	**-3.722309**	**0.953441**	**1.305289**
N	**2.178956**	**-1.073607**	**-2.521128**
N	**0.957040**	**-1.394840**	**-1.979920**
N	**1.703029**	**1.743819**	**-1.029884**
N	**2.798914**	**1.292296**	**-1.726954**
S	**-1.263025**	**-0.011740**	**1.869704**
S	**-2.182164**	**0.773565**	**-0.899097**
B	**3.233323**	**-0.197597**	**-1.780623**
H	**5.453484**	**-1.548704**	**-0.628331**
H	**3.223638**	**-1.563498**	**-4.303401**
H	**4.279524**	**2.178298**	**-2.964553**
H	**-3.094917**	**1.035457**	**3.300596**
H	**4.253079**	**-0.253753**	**-2.409602**
H	**0.971300**	**-3.037261**	**-4.847662**
H	**5.111115**	**-2.416272**	**1.955556**
H	**2.900146**	**4.491334**	**-2.423568**
H	**-4.736150**	**1.631088**	**2.996554**
H	**-4.307613**	**2.110859**	**-0.334874**
H	**-5.393453**	**2.178378**	**1.066730**
H	**-6.427911**	**0.956171**	**-0.870795**
H	**-5.103804**	**-0.228277**	**-0.844094**
H	**-6.250427**	**-0.135727**	**0.518372**
H	**-1.571705**	**-2.830137**	**-4.675698**
H	**-3.738496**	**-3.957305**	**-4.275567**
H	**-4.407196**	**-4.598673**	**-1.960285**
H	**-2.873715**	**-4.105668**	**-0.055808**
H	**-0.694604**	**-3.018608**	**-0.461922**
H	**0.522847**	**2.865014**	**1.255643**
H	**-1.154975**	**4.354616**	**2.285515**
H	**-2.036228**	**6.318007**	**1.024896**
H	**-1.225328**	**6.755637**	**-1.292571**
H	**0.434461**	**5.243456**	**-2.334209**
H	**3.223764**	**-3.596088**	**3.286812**
H	**2.204764**	**-3.889579**	**5.523937**
H	**0.825890**	**-2.065710**	**6.520512**
H	**0.494205**	**0.056440**	**5.253010**
H	**1.551494**	**0.361723**	**3.038504**
H	**-4.750317**	**-0.528088**	**4.273160**
H	**-5.544654**	**-0.747935**	**2.699985**
H	**-3.879593**	**-1.333324**	**2.950113**

Model 20

98

Cd	-0.744677	0.133757	0.107364
N	2.093290	1.221549	-0.434822
N	0.971913	1.752912	0.166487
C	1.082461	3.133050	0.075691
C	2.284713	3.438959	-0.659016
C	2.881193	2.235001	-0.927096
O	-2.473925	-1.214268	0.676229
C	-3.729323	-1.027972	0.512917
C	-4.336755	0.154973	0.031057
C	-3.705951	1.352830	-0.374287
C	-4.613537	2.536890	-0.864129
C	-5.483711	3.036910	0.324677
C	0.212322	4.024718	0.723934
C	-0.808482	3.545292	1.715681
B	2.464451	-0.297010	-0.415241
N	2.165205	-0.922321	0.971823
C	2.907072	-1.883935	1.627645
C	2.188416	-2.352690	2.690404
C	0.946735	-1.612349	2.695399
N	0.945026	-0.762898	1.589804
C	-0.047054	-1.609895	3.677112
C	-1.152628	-0.592211	3.686925
N	0.339884	-0.798743	-1.788419
N	1.649073	-1.112474	-1.466223
C	1.954258	-2.376550	-1.922047
C	0.880579	-2.885986	-2.597785
C	-0.146435	-1.868903	-2.549421
C	-1.370207	-1.849972	-3.221734
C	-2.242062	-0.628162	-3.263312
O	-2.444286	1.571689	-0.371097
C	-3.741746	3.707988	-1.375555
C	-5.540211	2.068296	-2.021141
C	-1.870017	-3.054113	-3.974076
C	-0.036620	-2.610228	4.801349
C	0.307022	5.507263	0.493588
C	-4.661113	-2.231057	0.897813
C	-5.503584	-2.663919	-0.335554
C	-3.812943	-3.436085	1.367639
C	-5.614464	-1.804552	2.050270
H	3.910127	-2.110478	1.302182
H	3.824771	2.024558	-1.407483
H	2.928857	-2.806491	-1.742813
N	3.958762	-0.435572	-0.785387
H	2.524851	-3.075602	3.418890
H	2.686013	4.414863	-0.889034
H	0.841910	-3.834845	-3.112272
H	-5.418939	0.140645	-0.034988
H	-6.100225	3.888991	0.005026
H	-6.153996	2.253486	0.696800
H	-4.854560	3.368610	1.160793
H	-4.390908	4.521710	-1.725566
H	-3.092199	4.099987	-0.587059
H	-3.098318	3.395831	-2.205109
H	-6.140743	2.915391	-2.381041
H	-4.953561	1.686051	-2.866101
H	-6.231423	1.279221	-1.704944
H	-6.243758	-2.655029	2.348197
H	-5.046454	-1.478534	2.931199
H	-6.275933	-0.982819	1.752852
H	-6.131294	-3.527063	-0.073124
H	-6.163460	-1.862241	-0.685888
H	-4.855213	-2.958337	-1.170585
H	-4.475993	-4.274028	1.621344
H	-3.118017	-3.763975	0.587748
H	-3.216953	-3.186952	2.251597
H	-2.888450	-3.322062	-3.646149
H	-1.946590	-2.846343	-5.055564
H	-1.240493	-3.938518	-3.845458
H	-2.638964	-0.476560	-4.279776
H	-3.120571	-0.730299	-2.603193
H	-1.705566	0.276749	-2.966441
H	-1.557757	-0.467950	4.699721
H	-0.803706	0.387188	3.333851
H	-1.986568	-0.890297	3.032612
H	-1.006800	-3.129920	4.866009
H	0.739378	-3.372506	4.695225
H	0.104839	-2.112403	5.776021
H	-1.136806	4.365494	2.366638
H	-1.700437	3.138073	1.214916
H	-0.406875	2.740352	2.347253
H	-0.679067	5.924394	0.230624
H	0.621763	6.034726	1.411126
H	1.003512	5.775763	-0.305100
N	4.937956	-0.199387	0.141552
C	6.127374	-0.152169	-0.555900
C	5.853897	-0.338385	-1.966240
C	4.496144	-0.500669	-2.060018
H	3.866043	-0.645987	-2.925104
H	6.556944	-0.354251	-2.786849
C	7.361407	0.052101	0.092922
C	8.656842	0.101371	-0.665320
C	7.438708	0.230538	1.581961
H	7.942901	1.177721	1.839425
H	6.449610	0.226177	2.044848
H	8.045914	-0.567082	2.045430
H	9.172619	1.064616	-0.507150
H	9.357097	-0.673048	-0.306040
H	8.532801	-0.037209	-1.742718

Model 21

89

Cd	**-0.226671**	**-0.352720**	**0.204251**
C	**0.239066**	**-1.801899**	**-3.199231**
C	**0.584958**	**-3.017212**	**-2.579025**
C	**1.553131**	**-3.832596**	**-3.198384**
C	**2.157905**	**-3.443296**	**-4.395824**
C	**1.808807**	**-2.228861**	**-4.998966**
C	**0.847989**	**-1.410571**	**-4.393966**
C	**-0.064971**	**-3.462713**	**-1.332716**
N	**-0.502722**	**-2.606521**	**-0.380004**
N	**-1.092772**	**-3.361910**	**0.604821**
C	**-1.021568**	**-4.677873**	**0.271209**
C	**-0.372585**	**-4.790782**	**-0.947328**
O	**-0.241474**	**1.475687**	**-1.029849**
C	**0.785292**	**2.152692**	**-1.430049**
C	**2.138688**	**1.806705**	**-1.267419**
C	**2.683372**	**0.644501**	**-0.655246**
C	**4.231423**	**0.408370**	**-0.649950**
B	**-1.728297**	**-2.756236**	**1.886066**
N	**-0.666484**	**-2.073333**	**2.799425**
C	**-0.235395**	**-2.487238**	**4.019474**
C	**0.633204**	**-1.534597**	**4.527940**
C	**0.689350**	**-0.516189**	**3.544989**
N	**-0.097042**	**-0.859740**	**2.497427**
C	**1.404041**	**0.770159**	**3.624316**
C	**0.886395**	**1.934128**	**3.024336**
C	**1.553827**	**3.155498**	**3.144091**
C	**2.745727**	**3.241666**	**3.872933**
C	**3.267566**	**2.092437**	**4.479435**
C	**2.604414**	**0.869483**	**4.355005**
C	**0.399788**	**3.468905**	**-2.186711**
O	**2.008694**	**-0.285868**	**-0.103796**
N	**-2.670038**	**-0.666352**	**0.684724**
C	**-3.835904**	**0.024028**	**0.702133**
C	**-4.754974**	**-0.599016**	**1.582319**
C	**-4.089444**	**-1.706506**	**2.077236**
N	**-2.843189**	**-1.740359**	**1.534188**
C	**-4.114902**	**1.196250**	**-0.150699**
C	**-3.711793**	**1.237057**	**-1.497687**
C	**-4.075687**	**2.308589**	**-2.317285**
C	**-4.840007**	**3.364088**	**-1.806818**
C	**-5.238372**	**3.340547**	**-0.464802**
C	**-4.882142**	**2.265467**	**0.353617**
H	**-0.592194**	**-3.415029**	**4.443603**
H	**-1.447291**	**-5.432431**	**0.916892**
H	**-4.413190**	**-2.477818**	**2.761572**
H	**-2.213122**	**-3.658457**	**2.509753**
H	**1.117225**	**-1.541071**	**5.493700**
H	**-0.185437**	**-5.695613**	**-1.506990**
H	**-5.777197**	**-0.305951**	**1.774368**
H	**-0.056869**	**1.887590**	**2.487358**
H	**1.134745**	**4.042979**	**2.676337**
H	**3.261174**	**4.194373**	**3.969984**
H	**4.195380**	**2.147043**	**5.044268**
H	**3.026896**	**-0.021445**	**4.812351**
H	**1.845143**	**-4.767226**	**-2.726332**
H	**2.907561**	**-4.084351**	**-4.853885**
H	**2.280103**	**-1.924215**	**-5.930539**
H	**0.565026**	**-0.467898**	**-4.855781**
H	**-0.524913**	**-1.169329**	**-2.756491**
H	**-5.192131**	**2.253118**	**1.395737**
H	**-5.827150**	**4.158324**	**-0.055417**
H	**-5.124089**	**4.195099**	**-2.448312**
H	**-3.769738**	**2.315472**	**-3.360417**
H	**-3.135475**	**0.411759**	**-1.904563**
H	**2.854777**	**2.504951**	**-1.672316**
C	**4.510695**	**-0.838024**	**-1.538145**
C	**5.058922**	**1.602689**	**-1.182435**
C	**4.672292**	**0.101184**	**0.807515**
C	**-0.537546**	**4.300967**	**-1.267274**
C	**1.605970**	**4.350356**	**-2.590566**
C	**-0.369490**	**3.060694**	**-3.475844**
H	**5.744798**	**-0.137231**	**0.828273**
H	**4.498627**	**0.962640**	**1.465008**
H	**4.114484**	**-0.750946**	**1.206773**
H	**5.583186**	**-1.077823**	**-1.516597**
H	**3.949936**	**-1.704243**	**-1.172448**
H	**4.220477**	**-0.656707**	**-2.581189**
H	**6.128299**	**1.362012**	**-1.113476**
H	**4.839436**	**1.820315**	**-2.234859**
H	**4.885022**	**2.513369**	**-0.595973**
H	**1.239467**	**5.256019**	**-3.092214**
H	**2.190023**	**4.667516**	**-1.718151**
H	**2.278160**	**3.836621**	**-3.288335**
H	**-0.723043**	**3.957052**	**-4.004264**
H	**0.281197**	**2.497559**	**-4.158801**
H	**-1.234490**	**2.439667**	**-3.226279**
H	**-0.873666**	**5.204746**	**-1.793941**
H	**-1.415660**	**3.719130**	**-0.974315**
H	**-0.010638**	**4.616567**	**-0.356416**

Model 22

85

Cd	**0.070518**	**-0.678435**	**0.278650**
C	**-4.007855**	**2.152629**	**0.826438**
C	**-2.873098**	**2.864449**	**0.392329**
C	**-2.972016**	**4.263798**	**0.263251**
C	**-4.168769**	**4.926958**	**0.549115**
C	**-5.292832**	**4.203981**	**0.965585**
C	**-5.206267**	**2.813268**	**1.104115**
C	**-1.608787**	**2.089265**	**0.104479**
C	**-0.584714**	**2.699962**	**-0.660675**
C	**0.666405**	**2.162233**	**-1.019097**
O	**1.128244**	**0.991944**	**-0.728329**
N	**-1.495057**	**-2.157966**	**-0.706962**
C	**-2.567243**	**-2.102307**	**-1.531983**
C	**-3.381290**	**-3.242915**	**-1.323744**
C	**-2.731330**	**-3.984879**	**-0.351119**
N	**-1.600345**	**-3.324538**	**0.013332**
C	**-2.759079**	**-1.037661**	**-2.533909**
C	**-1.663318**	**-0.441728**	**-3.186701**
C	**-1.860804**	**0.527386**	**-4.173507**
C	**-3.156629**	**0.915829**	**-4.532669**
C	**-4.255121**	**0.328526**	**-3.893376**
C	**-4.058317**	**-0.637849**	**-2.904170**
B	**-0.524129**	**-3.802066**	**1.021363**
N	**-0.519154**	**-2.973701**	**2.341255**
C	**-0.609351**	**-3.478455**	**3.599791**
C	**-0.320339**	**-2.470671**	**4.503236**
C	**-0.048565**	**-1.324846**	**3.716438**
N	**-0.174901**	**-1.641253**	**2.403960**
C	**0.338131**	**0.010259**	**4.212674**
C	**-0.112056**	**1.195036**	**3.602915**
C	**0.265297**	**2.441715**	**4.111799**
C	**1.088681**	**2.528476**	**5.239650**
C	**1.535283**	**1.355085**	**5.860036**
C	**1.164200**	**0.108499**	**5.351472**
N	**1.505621**	**-2.630102**	**-0.088260**
N	**0.891647**	**-3.772716**	**0.385446**
C	**1.759776**	**-4.817384**	**0.333027**
C	**2.962646**	**-4.366356**	**-0.179516**
C	**2.765397**	**-2.987692**	**-0.439529**
C	**3.754683**	**-2.074551**	**-1.044439**
C	**5.119109**	**-2.215340**	**-0.716098**
C	**6.089423**	**-1.417150**	**-1.326147**
C	**5.715035**	**-0.463319**	**-2.280886**
C	**4.363657**	**-0.311855**	**-2.611248**
C	**3.391915**	**-1.107521**	**-1.998259**
O	**-1.558101**	**0.907728**	**0.592528**
H	**-0.870918**	**-4.514970**	**3.757255**
H	**1.454155**	**-5.802365**	**0.655797**
H	**-2.978628**	**-4.939201**	**0.091228**
H	**-0.781241**	**-4.934908**	**1.317533**
H	**-0.334032**	**-2.531770**	**5.581619**
H	**3.848026**	**-4.949280**	**-0.387993**
H	**-4.283533**	**-3.508965**	**-1.855139**
H	**-0.777254**	**1.139871**	**2.747026**
H	**-0.095877**	**3.346538**	**3.629670**
H	**1.378186**	**3.500182**	**5.633391**
H	**2.179159**	**1.410232**	**6.734896**
H	**1.531964**	**-0.798361**	**5.825039**
H	**5.414227**	**-2.947149**	**0.031671**
H	**7.135753**	**-1.537990**	**-1.054685**
H	**6.469257**	**0.154683**	**-2.763186**
H	**4.062348**	**0.426274**	**-3.349522**
H	**2.348888**	**-0.986680**	**-2.270893**
H	**-4.916391**	**-1.077670**	**-2.402096**
H	**-5.265849**	**0.628309**	**-4.160272**
H	**-3.309492**	**1.667096**	**-5.304158**
H	**-1.000775**	**0.970245**	**-4.670046**
H	**-0.655195**	**-0.762065**	**-2.940115**
H	**-0.772550**	**3.707569**	**-1.002499**
H	**-2.109162**	**4.848791**	**-0.040371**
H	**-4.221737**	**6.008904**	**0.451791**
H	**-6.224729**	**4.720501**	**1.184769**
H	**-6.073812**	**2.243624**	**1.430187**
H	**-3.928819**	**1.076195**	**0.937539**
C	**1.606432**	**3.040139**	**-1.808331**
C	**1.147851**	**3.989088**	**-2.742651**
C	**2.050453**	**4.782703**	**-3.457048**
C	**3.427562**	**4.651359**	**-3.240176**
C	**3.894287**	**3.708976**	**-2.315424**
C	**2.993143**	**2.902635**	**-1.615019**
H	**0.082723**	**4.090017**	**-2.932565**
H	**1.678890**	**5.499841**	**-4.185565**
H	**4.129403**	**5.274780**	**-3.789771**
H	**4.962245**	**3.600541**	**-2.139687**
H	**3.350335**	**2.160369**	**-0.908400**

Model 23

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Cd	**-0.387350**	**-0.205688**	**0.290449**
C	**2.269494**	**1.884677**	**2.291447**
C	**2.406657**	**0.668151**	**2.987075**
C	**3.695775**	**0.257653**	**3.378404**
C	**4.814942**	**1.037853**	**3.077355**
C	**4.666925**	**2.243633**	**2.381055**
C	**3.390266**	**2.663245**	**1.989454**
C	**1.226393**	**-0.133954**	**3.359592**
C	**-0.288435**	**-1.323302**	**4.480246**
C	**0.992511**	**-0.804583**	**4.583442**
C	**1.555224**	**1.581487**	**-1.551887**
C	**-1.914033**	**-3.260115**	**-0.425937**
C	**-2.796162**	**-4.105589**	**0.287543**
C	**-2.924840**	**-3.532621**	**1.541110**
C	**-1.465225**	**-3.438493**	**-1.821085**
C	**-0.129704**	**-3.227615**	**-2.207375**
C	**0.267082**	**-3.434100**	**-3.532261**
C	**-0.658946**	**-3.860972**	**-4.490267**
C	**-1.989611**	**-4.082910**	**-4.114481**
C	**-2.389202**	**-3.874729**	**-2.792414**
C	**2.589892**	**-0.608686**	**-1.032794**
C	**-4.146912**	**0.384255**	**2.560699**
C	**-4.526369**	**1.422644**	**1.729794**
C	**-3.452828**	**1.590731**	**0.821357**
C	**-3.386723**	**2.588833**	**-0.264674**
C	**-4.556333**	**2.891608**	**-0.992402**
C	**-4.542306**	**3.858864**	**-1.999603**
C	**-3.358152**	**4.543620**	**-2.299677**
C	**-2.192509**	**4.252379**	**-1.583038**
C	**-2.206344**	**3.287061**	**-0.572319**
C	**2.617004**	**0.671817**	**-1.623304**
C	**3.846599**	**-1.520537**	**-1.234319**
C	**1.736736**	**2.954753**	**-2.274679**
N	**0.140027**	**-0.264941**	**2.561134**
N	**-0.792344**	**-0.996143**	**3.261894**
N	**-2.167817**	**-2.405737**	**1.585882**
N	**-1.536663**	**-2.229781**	**0.371690**
N	**-2.476775**	**0.690269**	**1.098471**
N	**-2.917794**	**-0.052197**	**2.178575**
O	**0.424642**	**1.475053**	**-0.983878**
O	**1.666238**	**-1.160263**	**-0.380023**
B	**-2.203065**	**-1.325084**	**2.709923**
H	**-3.496745**	**-3.842811**	**2.403800**
H	**-4.656282**	**-0.073535**	**3.396551**
H	**-0.882070**	**-1.882478**	**5.189135**
H	**-2.852195**	**-1.772105**	**3.612191**
H	**-3.239344**	**-5.025879**	**-0.063996**
H	**-5.429961**	**2.012080**	**1.784957**
H	**1.650608**	**-0.849485**	**5.438993**
H	**0.602433**	**-2.927487**	**-1.465666**
H	**1.305721**	**-3.273037**	**-3.809471**
H	**-0.346989**	**-4.023025**	**-5.519451**
H	**-2.718090**	**-4.411500**	**-4.852099**
H	**-3.427275**	**-4.031502**	**-2.510015**
H	**-5.474043**	**2.350188**	**-0.776694**
H	**-5.452861**	**4.071990**	**-2.554928**
H	**-3.344584**	**5.295517**	**-3.085341**
H	**-1.268265**	**4.778158**	**-1.806693**
H	**-1.298283**	**3.082069**	**-0.016699**
H	**3.819264**	**-0.685349**	**3.904783**
H	**5.803391**	**0.701498**	**3.381140**
H	**5.537936**	**2.851787**	**2.148587**
H	**3.263778**	**3.604447**	**1.459841**
H	**1.278303**	**2.234826**	**2.017034**
H	**3.512159**	**0.972555**	**-2.150698**
F	**4.234175**	**-2.093217**	**-0.067829**
F	**3.543935**	**-2.534849**	**-2.109041**
F	**4.927042**	**-0.860114**	**-1.749450**
F	**2.999682**	**3.161708**	**-2.753680**
F	**0.881390**	**3.060581**	**-3.329864**
F	**1.459827**	**3.988530**	**-1.420347**

Model 24

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Cd	**-0.068273**	**-0.000162**	**0.526531**
C	**1.589326**	**-2.226224**	**-2.861772**
N	**0.964111**	**-1.280207**	**-2.118841**
N	**1.063933**	**-1.606764**	**-0.780408**
C	**1.760041**	**-2.768243**	**-0.701703**
C	**2.108308**	**-3.187780**	**-2.008152**
B	**0.270080**	**0.000634**	**-2.657275**
N	**0.964240**	**1.281030**	**-2.117975**
N	**1.063278**	**1.606862**	**-0.779331**
C	**1.759569**	**2.768058**	**-0.699656**
C	**2.108248**	**3.188523**	**-2.005698**
C	**1.590181**	**2.227199**	**-2.860099**
O	**-0.479099**	**1.117719**	**2.568014**
C	**-0.599470**	**0.000935**	**3.177241**
C	**-0.934916**	**0.000790**	**4.663741**
C	**2.072911**	**3.476236**	**0.620137**
C	**0.766965**	**4.064368**	**1.229802**
C	**2.074231**	**-3.477564**	**0.617339**
C	**3.062816**	**-4.644721**	**0.356546**
N	**-1.773229**	**0.000075**	**-1.061413**
N	**-1.251874**	**0.000767**	**-2.338399**
C	**-2.266391**	**0.000924**	**-3.237215**
C	**-3.470247**	**-0.000216**	**-2.546986**
C	**-3.123835**	**0.000005**	**-1.175165**
C	**-4.060984**	**0.000180**	**0.033470**
C	**-3.822782**	**-1.270435**	**0.898065**
O	**-0.471819**	**-1.116030**	**2.569582**
C	**2.731926**	**-2.496717**	**1.626820**
C	**0.768405**	**-4.064107**	**1.228790**
C	**2.727251**	**2.493590**	**1.630026**
C	**3.063718**	**4.641964**	**0.361488**
C	**-3.830371**	**1.276381**	**0.892006**
C	**-5.534735**	**-0.005309**	**-0.449669**
H	**1.624379**	**-2.145186**	**-3.938880**
H	**1.625711**	**2.146785**	**-3.937252**
H	**-2.060872**	**0.001465**	**-4.298170**
H	**0.384459**	**0.001041**	**-3.850784**
H	**2.665709**	**-4.067839**	**-2.293169**
H	**2.665517**	**4.068912**	**-2.289892**
H	**-4.460250**	**-0.000525**	**-2.978797**
H	**-4.520256**	**-1.279163**	**1.746868**
H	**-3.991245**	**-2.180204**	**0.307869**
H	**-2.805075**	**-1.310987**	**1.300307**
H	**-4.528538**	**1.285330**	**1.740236**
H	**-2.813284**	**1.324594**	**1.294786**
H	**-4.003623**	**2.182237**	**0.297196**
H	**-6.206091**	**-0.005700**	**0.417936**
H	**-5.764739**	**0.882290**	**-1.051701**
H	**-5.759244**	**-0.896557**	**-1.048370**
H	**3.300630**	**5.138905**	**1.310355**
H	**4.003299**	**4.283625**	**-0.077115**
H	**2.634466**	**5.395270**	**-0.310210**
H	**1.001947**	**4.612319**	**2.152919**
H	**0.292569**	**4.762756**	**0.528417**
H	**0.051225**	**3.277059**	**1.480980**
H	**2.999598**	**3.032174**	**2.547633**
H	**2.040269**	**1.690919**	**1.914497**
H	**3.636933**	**2.046103**	**1.210392**
H	**1.004028**	**-4.612916**	**2.151238**
H	**0.054244**	**-3.275844**	**1.481555**
H	**0.291816**	**-4.761386**	**0.527783**
H	**3.005076**	**-3.036516**	**2.543490**
H	**3.641611**	**-2.050426**	**1.205899**
H	**2.046817**	**-1.693189**	**1.913216**
H	**3.300476**	**-5.142509**	**1.304794**
H	**2.631366**	**-5.397034**	**-0.314863**
H	**4.002259**	**-4.287600**	**-0.083349**
H	**-0.544503**	**-0.898524**	**5.147204**
H	**-0.546033**	**0.900975**	**5.146843**
H	**-2.027216**	**0.000041**	**4.772046**

Model 25

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Cd	**-0.000089**	**-0.000605**	**0.000051**
O	**-2.209485**	**-0.398832**	**-0.230848**
O	**-0.629746**	**2.072539**	**-0.705709**
O	**0.083806**	**-0.647583**	**-2.418703**
O	**2.209406**	**0.398861**	**0.224649**
O	**0.632031**	**-2.071945**	**0.709925**
O	**-0.089565**	**0.645732**	**2.419219**
H	**-0.856406**	**-0.528977**	**-2.651760**
H	**-4.855764**	**4.301289**	**-1.158098**
H	**-4.427578**	**4.502763**	**0.548785**
H	**-5.983237**	**3.768802**	**0.102767**
H	**-2.757829**	**4.542363**	**-1.034295**
H	**-1.330908**	**4.209176**	**-2.006056**
H	**-1.062273**	**3.911057**	**1.779549**
H	**-2.341154**	**5.130606**	**1.586188**
H	**-0.703109**	**5.627631**	**2.045707**
H	**0.935872**	**4.966994**	**-1.291134**
H	**0.909383**	**3.830731**	**0.066748**
H	**1.205008**	**5.561741**	**0.362089**
H	**-0.950867**	**6.704311**	**-1.573707**
H	**-0.609902**	**7.269540**	**0.073731**
H	**-2.260213**	**6.794031**	**-0.376365**
H	**-3.371069**	**-2.217718**	**0.076026**
H	**-4.617642**	**-4.325765**	**0.414441**
H	**-7.083775**	**-4.290527**	**0.798096**
H	**-8.278292**	**-2.097131**	**0.839012**
H	**-7.021261**	**0.015361**	**0.497763**
H	**1.929490**	**-0.045403**	**-3.036545**
H	**0.670561**	**1.187344**	**-3.259129**
H	**1.356168**	**0.215232**	**-5.476798**
H	**-0.335850**	**-0.194549**	**-5.135336**
H	**0.939268**	**-1.418540**	**-4.904378**
H	**0.849350**	**0.524391**	**2.656015**
H	**4.862089**	**-4.292507**	**1.178837**
H	**4.434493**	**-4.504654**	**-0.526970**
H	**5.988829**	**-3.765516**	**-0.084985**
H	**2.761712**	**-4.538344**	**1.049745**
H	**1.334051**	**-4.203039**	**2.019492**
H	**1.071018**	**-3.918047**	**-1.767591**
H	**2.349354**	**-5.137086**	**-1.567614**
H	**0.712100**	**-5.635487**	**-2.028541**
H	**-0.932438**	**-4.963741**	**1.303405**
H	**-0.904455**	**-3.832906**	**-0.058983**
H	**-1.198722**	**-5.565288**	**-0.347741**
H	**0.954316**	**-6.699635**	**1.595185**
H	**0.616634**	**-7.270751**	**-0.050889**
H	**2.265890**	**-6.792887**	**0.400543**
H	**3.368794**	**2.217312**	**-0.097865**
H	**4.612943**	**4.324037**	**-0.452230**
H	**7.079298**	**4.288791**	**-0.835101**
H	**8.276485**	**2.096532**	**-0.858360**
H	**7.021841**	**-0.014610**	**-0.500983**
H	**-1.939320**	**0.048774**	**3.030141**
H	**-0.684427**	**-1.187242**	**3.258030**
H	**-1.377563**	**-0.211257**	**5.472395**
H	**0.317687**	**0.191302**	**5.138012**
H	**-0.951356**	**1.420344**	**4.900714**
N	**-4.433983**	**0.277140**	**0.067693**
N	**-5.181347**	**1.462564**	**0.085369**
N	**4.434713**	**-0.276208**	**-0.070744**
N	**5.183479**	**-1.460796**	**-0.081266**
C	**-3.087481**	**0.531200**	**-0.166802**
C	**-2.980008**	**1.971135**	**-0.325886**
C	**-4.339692**	**2.449601**	**-0.148145**
C	**-4.925094**	**3.838346**	**-0.166187**
C	**-1.763073**	**2.656441**	**-0.636971**
C	**-0.885575**	**5.097834**	**-0.069142**
C	**-1.742822**	**4.147818**	**-0.987592**
C	**-1.274244**	**4.926364**	**1.421776**
C	**0.633486**	**4.842872**	**-0.242006**
C	**-1.197670**	**6.551812**	**-0.514116**
C	**-5.115026**	**-0.958824**	**0.265221**
C	**-4.438247**	**-2.193955**	**0.243262**
C	**-5.154502**	**-3.379983**	**0.436057**
C	**-6.535964**	**-3.362832**	**0.651321**
C	**-7.203758**	**-2.132291**	**0.673466**
C	**-6.507067**	**-0.937717**	**0.483322**
C	**0.899870**	**0.118775**	**-3.366025**
C	**0.699773**	**-0.353442**	**-4.804500**
C	**3.088490**	**-0.530475**	**0.165555**
C	**2.982683**	**-1.969687**	**0.332296**
C	**4.343145**	**-2.447522**	**0.157901**
C	**4.930746**	**-3.835236**	**0.184197**
C	**1.765995**	**-2.654742**	**0.645144**
C	**0.890964**	**-5.098463**	**0.084923**
C	**1.746428**	**-4.144884**	**1.000989**
C	**1.282148**	**-4.932155**	**-1.405942**
C	**-0.628496**	**-4.843669**	**0.254273**
C	**1.202984**	**-6.550709**	**0.535533**
C	**5.114286**	**0.959040**	**-0.276904**
C	**4.435986**	**2.193459**	**-0.264909**
C	**5.150962**	**3.378780**	**-0.466605**
C	**6.532541**	**3.361605**	**-0.681346**
C	**7.201831**	**2.131756**	**-0.693517**
C	**6.506477**	**0.937928**	**-0.494136**
C	**-0.911441**	**-0.118054**	**3.363674**
C	**-0.715766**	**0.354226**	**4.802639**

Model 26

99			
Cd	-0.124225	-0.036634	-0.018780
C	-3.346309	3.690284	1.145300
C	-3.577907	2.985214	-0.226579
C	-3.041727	3.870609	-1.385404
C	-3.665495	5.284238	-1.357161
C	-3.447138	5.980528	0.004604
C	-3.961137	5.108125	1.171225
C	-2.916439	1.598801	-0.220253
C	-0.281798	-0.703448	3.454522
C	-0.045124	-0.175489	4.869137
C	2.893606	0.820232	0.040301
C	3.454410	-0.508069	-0.163058
C	4.831407	-0.244988	-0.557491
C	2.690503	-1.705144	0.067778
C	3.953830	3.136339	-0.116871
C	5.189265	3.799101	-0.257319
C	5.248535	5.192029	-0.188830
C	4.089112	5.948722	0.020136
C	2.864659	5.287872	0.158777
C	2.784356	3.892778	0.092215
C	5.952724	-1.131660	-1.036361
C	3.247358	-3.144868	0.161510
C	3.672164	-3.771197	-1.197326
C	4.014700	-5.270416	-1.026632
C	5.080283	-5.496543	0.069448
C	4.648190	-4.873205	1.415965
C	4.304692	-3.370479	1.278087
C	0.372524	0.754348	-3.438000
C	0.361853	0.270120	-4.886918
C	-3.123283	-0.939053	-0.082437
C	-5.096423	0.191639	0.190055
C	-3.679481	0.401430	-0.048936
C	-4.236690	-3.221381	0.177881
C	-5.481844	-3.857156	0.354135
C	-5.554242	-5.249699	0.417519
C	-4.398931	-6.032990	0.307522
C	-3.164998	-5.398835	0.132874
C	-3.071047	-4.004605	0.067005
C	-6.238387	1.161216	0.355297
O	-1.648723	1.611724	-0.364639
O	-0.171476	0.353934	2.451538
O	1.726355	1.208580	0.401957
O	1.430832	-1.667542	0.275351
O	0.052755	-0.323038	-2.499343
O	-1.928217	-1.358548	-0.272293
N	5.097503	1.047685	-0.576167
N	3.928759	1.713602	-0.201612
N	-4.196836	-1.798340	0.121107
N	-5.393421	-1.088475	0.290966
H	-0.845322	-0.652879	-2.691559
H	-2.112450	-3.524436	-0.069047
H	-2.256153	-5.990193	0.045675
H	-4.460559	-7.117446	0.357123
H	-6.523986	-5.723176	0.554081
H	-6.373666	-3.248761	0.440257
H	1.371283	1.088718	-3.143332
H	-0.327754	1.587304	-3.289762
H	0.645935	1.092708	-5.556893
H	-0.638474	-0.073430	-5.184017
H	1.070721	-0.554080	-5.028150
H	0.741887	0.704068	2.450975
H	6.195861	-1.937174	-0.339697
H	5.712027	-1.589328	-2.003356
H	6.841386	-0.507763	-1.170438
H	1.833250	3.391952	0.203259
H	1.952755	5.858459	0.320410
H	4.140491	7.033513	0.073818
H	6.083838	3.211184	-0.422396
H	-1.300920	-1.085466	3.343585
H	0.417198	-1.515165	3.210163
H	-0.177417	-0.986572	5.597914
H	0.975747	0.213893	4.981536
H	-0.752650	0.626844	5.109097
H	2.354990	-3.704058	0.474492
H	5.221360	-2.806242	1.073579
H	3.911629	-2.989252	2.230818
H	5.439408	-5.003869	2.167255
H	3.764953	-5.411682	1.793743
H	6.033256	-5.046564	-0.251606
H	5.269519	-6.571654	0.195816
H	4.361424	-5.681389	-1.985085
H	3.100104	-5.822888	-0.760339
H	4.541292	-3.251563	-1.612707
H	2.853167	-3.652201	-1.919610
H	-4.655066	2.871431	-0.368349
H	-1.950238	3.942757	-1.297860
H	-3.253711	3.384989	-2.348667
H	-3.237860	5.892274	-2.166592
H	-4.746543	5.213379	-1.558130
H	-2.371419	6.172232	0.143618
H	-3.945626	6.959970	0.015256
H	-3.736117	5.588626	2.133716
H	-5.058490	5.031480	1.109045
H	-2.263262	3.749407	1.324240
H	-3.768696	3.079876	1.955359
H	6.210979	5.686729	-0.299221
H	-6.438516	1.720792	-0.566666
H	-7.137847	0.593034	0.610528
H	-6.048391	1.888187	1.153067

Table S1 Et_2Cd $\delta(^{113}Cd)$ [$\sigma(CdMe_2)_{(g)}$ -$\sigma(CdEt_2)_{(g)}$, ppm] in gas phase calculated by using different NR-1[*F*/*B*] protocols. Geometries from OP2. Experimental value: -142.6 ppm[53]

Basis set/ Functional	DZVP;cc-pvdz	DZVP;6-31G(d,p)	DZVP;6-311G+	Sadleji;cc-pvdz	Sadleji;6-31G(d,p)	Sadleji;6-311G+
B3PW91	-140.2	-142.9	-132.8	-111.8	-109.3	-106.9
BLYP	-153.0	-155.4	-148.2	-123.6	-120.6	-120.0
PBEPBE	-153.6	-155.8	-147.215	-122.8	-119.8	-118.5
VSXC	-146.3	-147.5	-140.2	-116.4	-112.8	-111.4
THCTH	-144.0	-145.3	-137.2	-117.2	-114.0	-112.1
M06L	-119.2	-123.7	-115.4	-88.5	-85.1	-84.5
B97D	-145.7	-147.5	-134.0	-118.4	-115.2	-113.8
B3LYP	-142.6	-145.2	-137.2	-115.6	-113.3	-111.8
mPW1PW91	-138.0	-140.6	-131.4	-110.0	-107.4	-105.6
PBE1PBE	-140.3	-142.9	-133.3	-112.5	-110.2	-108.0
HSEH1PBE	-140.3	-142.9	-133.5	-112.2	-109.9	-107.7
TPSSH	-140.9	-143.3	-133.9	-110.7	-107.6	-106.1
M062X	-132.1	-135.5	-125.2	-109.7	-108.6	-104.8
THCTHhyb	-142.7	-145.0	-135.9	-115.0	-112.1	-110.3
LC-WPBE	-130.7	-134.0	-122.5	-103.5	-102.0	-97.8
CAM-B3LYP	-137.9	-140.6	-131.8	-112.3	-110.5	-107.8
WB97XD	-134.3	-137.2	-127.5	-107.7	-105.3	-102.6

Table S2 Calculated σ(^{113}Cd) used for the δ(^{113}Cd) of Table 2. In parentheses are given the spinorbit contributions according to the ZORA approximation.

		NR1-BLYP[a]	NR2-BLYP[b]	RS-BLYP[b]	SO1-BLYP[b]	NR3-BLYP	DC-BLYP
OP1							
	Me_2Cd	2902.5 3073.0 2926.4 3095.8	3007.8 3023.8 2986.9	2959.1 2951.3 2889.3	3370.5 (420.98) 3352.7 (414.63) 3286.6 (428.97)	2987.4	3671.8
	Et_2Cd	3057.9 3193.6 3079.4 3219.4	3155.3 3169.6 3132.9	3102.4 3090.1 3034.5	3522.0 (429.18) 3498.0 (421.62) 3443.1 (439.07)	3132.3	3827.1
OP2							
	Me_2Cd	2905.97 3077.05 2929.87 3099.30	3010.9 3026.6 2990.2	2961.8 2953.8 2892.4	3373.3 (421.48) 3355.8 (415.14) 3290.4 (429.60)	2990.8	3048.0
	Et_2Cd	3061.86 3197.99 3083.49 3223.35	3159.2 3173.0 3136.9	3105.7 3093.5 3038.4	3525.7 (429.63) 3502.2 (422.27) 3447.8 (439.80)	3136.2	3183.3
OP3							
	Me_2Cd	2959.1 3128.2 2983.7 3151.1	3065.2 3080.8 3044.4	3018.8 3011.7 2951.6	3431.3 (422.31) 3414.8 (416.33) 3351.8 (431.51)	3044.7	3738.7
	Et_2Cd	3109.5 3242.6 3131.6 3270.7	3209.0 3222.4 3186.6	3159.2 3147.1 3093.2	3580.2 (430.69) 3556.9 (423.46) 3504.5 (441.52)	3185.9	3897.0
		NR1-B3LYP	**NR2-B3LYP**	**RS2-B3LYP**	**SO2-B3LYP**	**NR3-B3LYP**	**DC-B3LYP**
OP1							
	Me_2Cd	2974.1 3123.6 2993.8 3144.2	3067.8 3080.9 3046.5	3013.2 3003.1 2946.3	3455.8 (452.21) 3435.1 (445.17) 3381.7 (466.18)	3044.7	3754.5
	Et_2Cd	3119.3 3236.9 3136.4 3259.8	3205.6 3216.2 3183.1	3147.2 3131.5 3081.9	3597.6 (459.91) 3569.7 (451.81) 3527.5 (475.75)	3179.4	3900.3
OP2							
	Me_2Cd	2977.4 3127.6 2997.2 3147.6	3070.9 3083.7 3049.7	3016.1 3005.6 2949.3	3458.9 (452.34) 3437.8 (445.31) 3385.1 (466.35)	3048.0	3756.0
	Et_2Cd	3123.1	3209.4	3150.6	3601.1	3183.3	3904.0

		3241.3 3140.5 3263.7	3219.7 3186.9	3135.2 3085.6	(459.95) 3573.7 (452.07) 3531.6 (475.98)		
OP3							
	Me_2Cd	3048.4 3079.1 3176.1 3196.7	3122.6 3135.4 3101.8	3069.9 3060.4 3005.9	3514.8 (455.67) 3495.2 (448.01) 3445.5 (469.99)	3099.6	3819.74
	Et_2Cd	3186.0 3308.3 3220.3 3285.5	3256.68 3266.50 3234.66	3201.1 3185.7 3137.6	3654.1 (462.60) 3587.3 (454.89) 3626.9 (479.56)	3230.4	3962.6

[a] In the entry(are given the results obtained with, from top to bottom, DZVP (Cd)/6-31G(d,p) (H,C), Sadlej (Cd)/6-31G(d,p) (H,C), DZVP (Cd)/cc-pvdz (H,C) and Sadelj (Cd)/cc-pvdz (H,C)gaussian type basis, respectively.
[b] In the entry are given the esultes obtained with Slater type basis set of DZP, TZ2P and QZ4P quality, respectively.

Table S3 Calculated σ(^{113}Cd), for different d(Cd-C) bond distances (pm) and ϕ(Cd-C-C-H) dihedral angles (°) for Me_2Cd at SO[B3LYP/TZ2P;DZP], SC[B3LYP/TZ2P;DZP], NR-2[B3LYP/TZ2P;DZP] levels

SO **B3LYP/TZ2P**

d(Cd-C) → / ϕ (Cd-C-C-H) ↓	217	221	225	230	235
-20	3513.61	3592.88	3667.67	3755.04	3836.37
25	3513.00	3592.78	3667.64	3755.02	3836.37
55	3513.28	3593.06	3667.91	3755.25	3836.62
85	3514.04	3593.71	3668.49	3755.76	3837.06
145	3516.02	3595.61	3670.31	3757.55	3838.72
175	3515.92	3595.53	3670.25	3757.45	3838.65

B3LYP/DZP

	217	221	225	230	235
-20	3531.74	3610.18	3683.85	3769.92	3850.12
25	3532.21	3610.61	3684.23	3770.28	3850.43
55	3532.69	3611.04	3684.64	3770.61	3850.70
85	3532.75	3611.11	3684.73	3770.70	3850.82
145	3534.85	3613.07	3686.57	3772.41	3852.39
175	3535.02	3613.24	3686.70	3772.52	3852.47

SC **B3LYP/TZ2P**

	217	221	225	230	235
-20	3076.97	3152.99	3224.15	3306.98	3383.80
25	3077.12	3153.12	3224.27	3307.11	3383.91
55	3077.48	3153.45	3224.59	3307.40	3384.22
85	3077.97	3153.90	3225.03	3307.75	3384.52
145	3079.86	3155.73	3226.76	3309.44	3386.12
175	3079.92	3155.76	3226.80	3309.47	3386.15

B3LYP/DZP

	217	221	225	230	235
-20	3085.94	3161.22	3231.70	3313.78	3389.93
25	3086.31	3161.54	3231.99	3314.03	3390.14
55	3086.73	3161.93	3232.35	3314.35	3390.43
85	3086.94	3162.14	3232.56	3314.54	3390.62
145	3088.93	3164.01	3234.33	3316.22	3392.20
175	3089.06	3164.15	3234.45	3316.32	3392.28

NR **B3LYP/TZ2P**

	217	221	225	230	235
-20	3150.98	3222.47	3289.18	3366.54	3437.95
25	3151.56	3223.00	3289.67	3366.96	3438.33
55	3151.99	3223.38	3290.03	3367.32	3438.64
85	3152.04	3223.46	3290.10	3367.37	3438.71
145	3153.72	3225.04	3291.62	3368.78	3440.04
175	3153.95	3225.26	3291.79	3368.94	3440.16

B3LYP/DZP

	217	221	225	230	235
-20	3138.87	3210.55	3277.42	3354.97	3426.58
25	3138.97	3210.66	3277.54	3355.09	3426.70
55	3139.25	3210.93	3277.79	3355.32	3426.93
85	3139.75	3211.38	3278.19	3355.67	3427.21
145	3141.51	3213.07	3279.84	3357.27	3428.76
175	3141.48	3213.05	3279.82	3357.25	3428.74

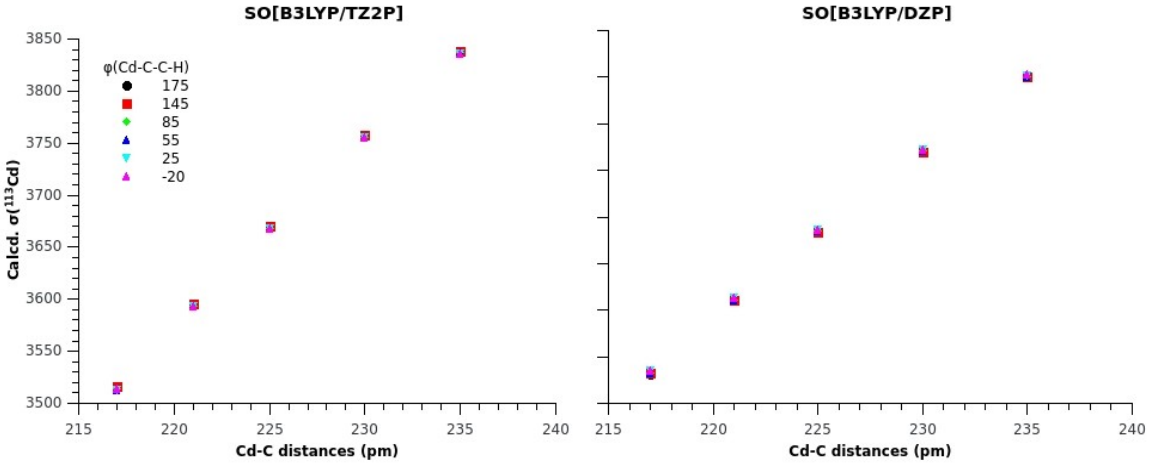

Figure S1 σ(^{113}Cd) dependence on Cd-C bond distance and Cd-C-C-H dihedral angles for Me_2Cd SO[B3LYP/TZ2P;DZP]

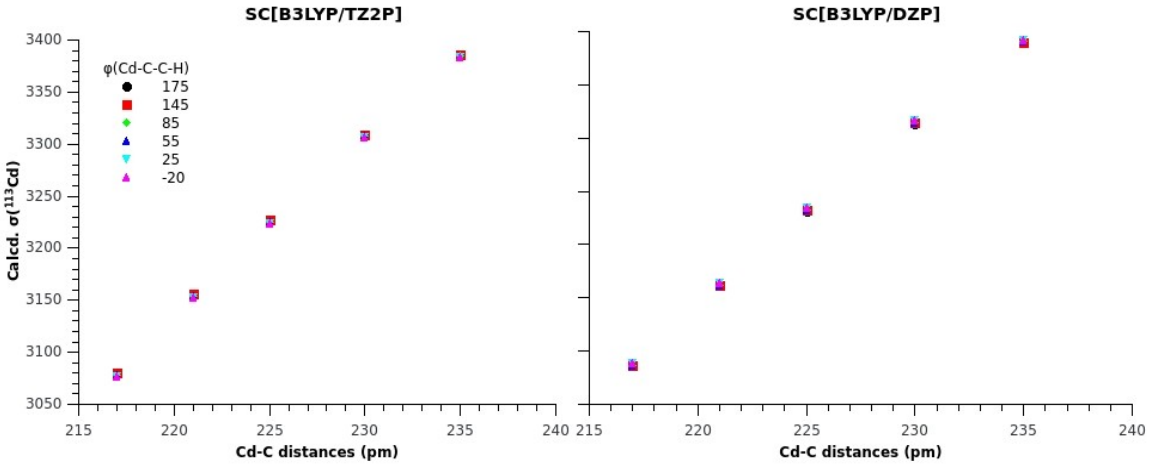

Figure S2 σ(^{113}Cd) dependence on Cd-C bond distance and Cd-C-C-H dihedral angles for Me_2Cd SC[B3LYP/TZ2P;DZP]

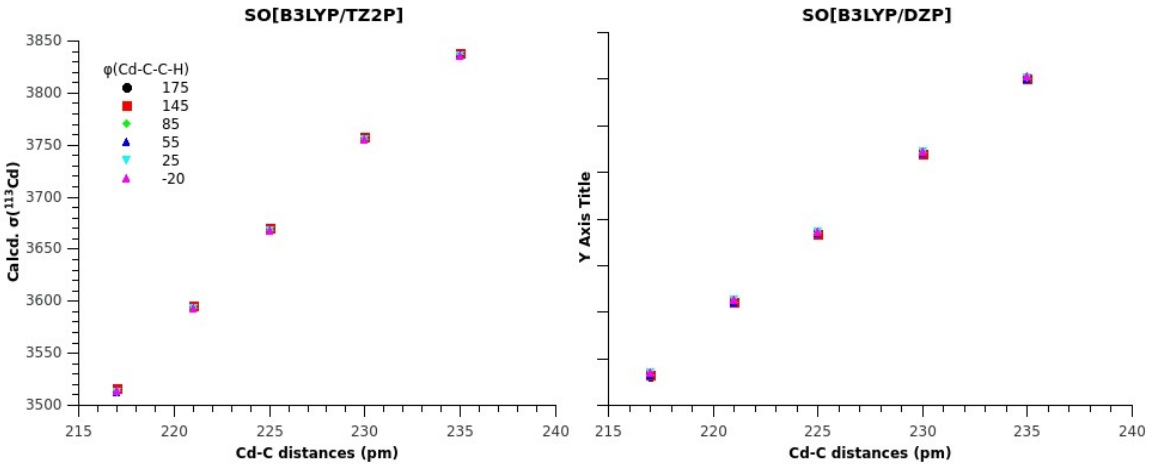

Figure S3 σ(^{113}Cd) dependence on Cd-C bond distance and Cd-C-C-H dihedral angles for Me_2Cd NR-2[B3LYP/TZ2P;DZP]

Table S4 Calculated and averaged σ_{iso}, σ_{xx}, σ_{yy} and σ_{zz} B3LYP/Sadleji (Cd);6-31G(d) (H,O,Cl)

snapshot	σ_{iso}	σ_{xx}	σ_{yy}	σ_{zz}
1	3817.74	3705.99	3867.53	3879.71
2	3864.86	3814.09	3824.70	3955.78
3	3840.85	3759.12	3813.48	3949.95
4	3896.89	3829.96	3898.62	3962.08
5	3806.63	3700.96	3851.45	3867.50
6	3861.54	3812.88	3879.07	3892.66
7	3894.01	3813.34	3850.62	4018.08
8	3841.20	3748.99	3864.43	3910.18
9	3751.40	3690.70	3714.85	3848.66
10	3805.30	3703.80	3829.48	3882.61
11	3868.11	3757.31	3818.25	4028.78
12	3798.33	3743.36	3800.12	3851.51
13	3873.81	3846.75	3878.52	3896.16
14	3849.89	3723.96	3814.54	4011.16
15	3801.62	3700.94	3773.40	3930.52
16	3866.11	3783.70	3887.64	3927.00
17	3788.86	3761.35	3793.13	3812.10
18	3857.56	3806.44	3878.19	3888.05
19	3834.53	3760.18	3853.19	3890.22
20	3874.68	3769.31	3855.43	3999.31
avg	**3839.70**	**3761.66**	**3837.3**	**3920.10**
StdDev	**38.373**			

Table S5 Calculated and averaged σ_{iso}, σ_{xx}, σ_{yy} and σ_{zz} for the 20 snapshots of the aqueous solution of $Cd(ClO_4)_2$ 1.0 M. B3PW91/Sadleji (Cd);6-31G(d) (H,O,Cl)

snapshot	σ_{iso}	σ_{xx}	σ_{yy}	σ_{zz}
1	3826.39	3711.26	3878.84	3889.08
2	3873.88	3821.41	3835.20	3965.03
3	3848.98	3765.17	3822.00	3959.77
4	3906.16	3837.72	3908.78	3971.98
5	3815.21	3708.19	3860.85	3876.59
6	3870.21	3819.95	3887.70	3902.98
7	3904.32	3823.03	3863.05	4026.89
8	3849.42	3755.36	3873.73	3919.17
9	3757.43	3695.43	3720.44	3856.43
10	3813.06	3710.43	3837.42	3891.33
11	3877.50	3764.76	3829.25	4038.50
12	3806.14	3752.04	3806.54	3859.83
13	3881.95	3854.71	3886.93	3904.21
14	3859.09	3732.80	3823.80	4020.68
15	3809.76	3710.32	3780.31	3938.64
16	3874.89	3790.99	3896.79	3936.90
17	3796.53	3768.30	3800.31	3820.98
18	3864.92	3812.41	3885.72	3896.63
19	3841.63	3764.60	3861.22	3899.06
20	3883.31	3776.51	3865.25	4008.18
avg	**3848.04**	**3768.77**	**3846.21**	**3929.14**
StdDev	**39.064**			

Table S6 Calculated and averaged σ_{iso}, σ_{xx}, σ_{yy} and σ_{zz} for the 20 snapshots of the aqueous solution of $Cd(ClO_4)_2$ 1.0 M. B3LYP/Sadleji (Cd);6-31G(d,p) (H,O,Cl)

snapshot	σ_{iso}	σ_{xx}	σ_{yy}	σ_{zz}
1	3815.17	3704.78	3864.37	3876.35
2	3861.91	3811.61	3821.57	3952.54
3	3838.39	3756.75	3810.84	3947.58
4	3893.60	3826.79	3895.02	3958.98
5	3804.07	3698.06	3849.32	3864.84
6	3859.44	3811.10	3876.70	3890.51
7	3891.19	3810.75	3848.08	4014.75
8	3838.86	3746.17	3862.40	3908.00
9	3749.46	3688.02	3712.91	3847.47
10	3802.57	3701.11	3826.30	3880.29
11	3865.28	3754.14	3816.04	4025.66
12	3795.76	3740.72	3797.82	3848.74
13	3870.73	3843.23	3875.29	3893.68
14	3848.02	3721.94	3812.60	4009.52
15	3798.68	3698.32	3770.61	3927.10
16	3863.19	3781.03	3884.51	3924.02
17	3786.75	3759.08	3791.05	3810.11
18	3855.19	3804.12	3875.72	3885.72
19	3831.53	3756.90	3849.91	3887.77
20	3872.70	3767.54	3853.51	3997.05
avg	**3837.12**	**3759.11**	**3834.73**	**3917.53**
StdDev	**38.219**			

Table S7Calculated and averaged σ_{iso}, σ_{xx}, σ_{yy} and σ_{zz} for the 20 snapshots of the aqueous solution of $Cd(ClO_4)_2$ 1.0 M. B3PW91/Sadleji (Cd);6-31G(d,p) (H,O,Cl)

snapshot	σ_{iso}	σ_{xx}	σ_{yy}	σ_{zz}
1	3823.88	3709.66	3876.20	3885.77
2	3870.82	3818.78	3832.00	3961.68
3	3846.45	3762.76	3819.35	3957.22
4	3902.74	3834.40	3905.10	3968.73
5	3812.55	3705.18	3858.48	3874.00
6	3870.35	3819.82	3886.90	3904.32
7	3900.41	3817.04	3859.41	4024.78
8	3846.75	3752.31	3871.28	3916.65
9	3755.42	3692.74	3718.38	3855.15
10	3810.20	3707.63	3834.18	3888.79
11	3874.40	3761.35	3826.71	4035.13
12	3803.41	3749.24	3804.14	3856.86
13	3878.77	3850.96	3883.64	3901.70
14	3856.24	3730.09	3820.99	4017.63
15	3806.81	3707.26	3777.54	3935.64
16	3871.79	3788.14	3893.54	3933.70
17	3794.19	3765.78	3798.00	3818.78
18	3862.35	3809.91	3883.08	3894.07
19	3839.00	3761.57	3858.79	3896.65
20	3135.67	1711.43	3832.15	3863.42
avg	**3843.50**	**3662.80**	**3841.99**	**3919.54**
StdDev	**38.99**			

[a] **Snapshot #20 has not been included in the average of the isotropic shielding.**

Table S8 Calculated and averaged σ_{iso}, σ_{xx}, σ_{yy} and σ_{zz} for the 20 snapshots of the aqueous solution of $Cd(ClO_4)_2$ 1.0 M. B3LYP/Sadleji (Cd);6-31+G(d,p) (H,O,Cl)

snapshot	σ_{iso}	σ_{xx}	σ_{yy}	σ_{zz}
1	3806.64	3692.53	3857.63	3869.77
2	3855.58	3802.73	3813.50	3950.50
3	3835.40	3755.58	3809.59	3941.03
4	3889.39	3825.33	3891.07	3951.75
5	3792.83	3680.23	3841.95	3856.32
6	3853.17	3801.52	3873.72	3884.27
7	3886.81	3804.31	3840.99	4015.13
8	3835.27	3742.51	3859.61	3903.69
9	3742.59	3683.14	3703.17	3841.47
10	3795.41	3692.14	3820.59	3873.50
11	3857.86	3746.65	3805.05	4021.88
12	3789.80	3731.83	3785.51	3852.05
13	3866.20	3836.89	3873.05	3888.67
14	3842.82	3719.36	3803.79	4005.31
15	3794.41	3694.50	3766.35	3922.38
16	3858.14	3776.71	3876.30	3921.41
17	3776.96	3746.88	3778.23	3805.75
18	3851.27	3802.43	3871.24	3880.15
19	3825.30	3751.25	3841.09	3883.55
20	3860.93	3756.43	3836.95	3989.40
avg	**3830.84**	**3752.15**	**3827.47**	**3912.90**
StdDev	**39.02**			

Table S9 Calculated and averaged σ_{iso}, σ_{xx}, σ_{yy} and σ_{zz} for the 20 snapshots of the aqueous solution of $Cd(ClO_4)_2$ 1.0 M. B3PW91/Sadleji (Cd);6-31+G(d,p) (H,O,Cl)

snapshot	σ_{iso}	σ_{xx}	σ_{yy}	σ_{zz}
1	3814.6314	3697.7229	3868.5894	3877.5818
2	3864.0154	3810.3265	3822.5278	3959.1920
3	3842.9164	3761.1961	3817.5326	3950.0206
4	3897.8275	3832.5224	3900.4005	3960.5595
5	3800.5122	3686.3902	3850.5369	3864.6095
6	3861.1355	3808.0461	3881.9608	3893.3996
7	3895.3402	3810.7806	3850.8535	4024.3865
8	3842.7312	3748.3432	3868.3565	3911.4940
9	3748.2746	3687.8386	3707.9242	3849.0609
10	3801.8354	3697.5732	3827.1263	3880.8066
11	3866.5637	3753.3001	3815.1760	4031.2149
12	3796.9637	3739.3868	3791.5979	3859.9065
13	3873.6447	3844.3479	3880.3969	3896.1893
14	3850.6909	3726.7121	3811.7333	4013.6274
15	3801.3802	3702.0367	3772.2303	3929.8735
16	3866.0390	3783.0782	3884.9230	3930.1157
17	3783.6401	3752.7595	3784.5248	3813.6359
18	3858.1287	3808.1294	3878.0407	3888.2159
19	3832.5849	3756.1940	3849.3296	3892.2310
20	3868.9092	3762.9631	3846.2184	3997.5462
avg	**3838.39**	**3758.48**	**3835.50**	**3921.18**
StdDev	**39.63**			

Table S10 Correlations at NR-1[F/*B*] [F=B3LYP,B3PW91; B=DZVP(Cd), 6-31G(d,p) levels of calculated δ(^{113}Cd) (ppm), wrt $Cd(ClO_4)_2$ and Me_2Cd, respectively, on OP2 geometries, and relevant statistical data. For the complete set of calculated δ(^{113}Cd) see Tables S14-S48.

Exptl. (wrt 1M $Cd(ClO_4)_2$)	Calcd		Exptl. (wrt $Me_2Cd_{(g)}$)	Calcd	
	B3LYP/ DZVP;6-31G(d,p)	B3PW91/ DZVP;6-31G(d,p)		B3LYP/ DZVP;6-31G(d,p)	B3PW91/ DZVP;6-31G(d,p)
77.1	**-7.27**	**0.75**	**-629.03**	**-863.99**	**-847.18**
82.1	**-2.76**	**5.46**	**-624.03**	**-859.48**	**-842.46**
76	**-8.27**	**-0.14**	**-630.13**	**-864.99**	**-848.06**
81.2	**6.52**	**14.67**	**-624.93**	**-850.21**	**-833.26**
59.1	**-6.66**	**1.85**	**-647.03**	**-863.39**	**-846.07**
200	**111.52**	**129.38**	**-506.13**	**-745.20**	**-718.55**
202.5	**110.77**	**131.14**	**-503.63**	**-745.96**	**-716.78**
193.8	**142.18**	**156.15**	**-512.33**	**-714.54**	**-691.77**
195.9	**147.35**	**164.48**	**-510.23**	**-709.37**	**-683.44**
218.3	**188.54**	**203.42**	**-487.83**	**-668.18**	**-644.51**
201.9	**118.55**	**136.89**	**-504.23**	**-738.17**	**-711.03**
198.3	**152.17**	**166.89**	**-507.83**	**-704.55**	**-681.03**
221.1	**192.27**	**207.12**	**-485.03**	**-664.45**	**-640.81**
353.6	**252.65**	**253.84**	**-352.53**	**-604.07**	**-594.08**
365.13	**263.59**	**264.83**	**-341.00**	**-593.13**	**-583.09**
352.13	**253.45**	**254.71**	**-354.00**	**-603.27**	**-593.22**
303.3	**273.24**	**282.51**	**-402.83**	**-583.48**	**-565.41**
265.67	**199.92**	**209.96**	**-440.46**	**-656.80**	**-637.97**
237.5	**160.63**	**173.05**	**-468.63**	**-696.09**	**-674.87**
168.2	**168.00**	**135.78**	**-537.93**	**-688.72**	**-712.14**
172.4	**125.73**	**152.71**	**-533.73**	**-730.99**	**-695.21**
155.2	**143.75**	**151.78**	**-550.93**	**-712.98**	**-696.14**
141.8	**137.84**	**144.93**	**-564.33**	**-718.88**	**-703.00**
148.1	**132.39**	**144.67**	**-558.03**	**-724.34**	**-703.26**
27.2	**-37.09**	**-30.44**	**-678.93**	**-893.82**	**-878.37**
26.3	**-38.03**	**-31.71**	**-679.83**	**-894.75**	**-879.63**
ME	101.54	100.30	ME	252.13	242.09
MAE	59.34	50.21	MAE	209.93	191.76
CMAE	28.19	28.66	CMAE	28.19	28.66
Slope	0.945	0.941	Slope	0.945	0.941
Int.	-49.35	-39.27	Int.	-238.77	-222.63

Table S11 Calculated Cd-N, Cd-O and Cd-S bond lengths (pm) for the models of Scheme 1 with OP2 and OP3 protocols. Averaged values.

Model	OPTIMIZATION PROTOCOL					
	OP2			OP3		
	Cd-N	Cd-O	Cd-S	Cd-N	Cd-O	Cd-S
1	238	232	-	238	234	-
2	239	231	-	240	233	-
3	238	231	-	239	234	-
4	238	230	-	239	234	-
5	240	231	-	239	234	-
6	240	-	-	243	-	-
7	240	-	-	242	-	-
8	238	-	-	241	-	-
9	238	-	-	241	-	-
10	237	-	-	239	-	-
11	239	-	-	243	-	-
12	238	-	-	241	-	-
13	237	-	-	239	-	-
14	-	-	261	-	-	261
15	-	-	259	-	-	260
16	-	-	259	-	-	261
17	226	-	-	228	-	-
18	235	-	267	236	-	270
19	238	-	264	242	-	265
20	234	225	-	234	225	-
21	236	222	-	241	224	-
22	235	222	-	239	226	-
23	235	227	-	237	231	-
24	232	233	-	235	236	-
25	-	245_{ax};225_{eq}	-	-	251_{ax};226_{eq}; 228_{eq}	-
26	-	243_{ax};245_{ax}; 225_{eq}	-	-	250_{ax}; 225_{eq};227_{eq}	-

Table S12 Calculated plane and dihedral angles for the models of Scheme 1 with OP2 and OP3 protocols.

Model	OPTIMIZATION PROTOCOL							
	OP2				OP3			
	N-Cd-N	***O-Cd-O-C***	***Cd-O-C-N***	***Cd-O-C-R'***	***N-Cd-N***	***O-Cd-O-C***	***Cd-O-C-N***	***Cd-O-C-R'***
1	179	158; -64; -111; -171	163; 155	168; 173	179	173; -54; -110; 155	175; 168	165; 172
2	178	171; -83; -95; 177	175;168	165; 172	178	-176; -86; -84; 170	180	162;166
3	179	-91; 164; -177; -98	155;161	172; 170	178	-142; -173; -177; -56	161; -177	174; 166
4	175	177; -115; -81; 163	177; -171	-176; 179	176	168; -113; -93; 174	167; 178	-167; -175
5	173	150; -55; -82; -112	170; 149	167; 179	172	-166; 130; -163; 69	161; 169	174; 166
	N-Cd-N (same ligand)	***C-N-Cd-N***	***Cd-N-N-B (same ligand)***		***N-Cd-N (same ligand)***	***C-N-Cd-N***	***Cd-N-N-B (same ligand)***	
6	82	-42	0		82	-41	0	
7	80; 81,82	-49	-12;-14; -29		80;81;83	-45	-9;-27;-28	
8	81;82	-44	0		82	-43	0	
9	81	-40	0		81	-45	0	
10	80;81	-41	10; 22; 6		80;81	-39	10; 22; 7	
11	82	-42	0		81	-41	0	
12	81	-45	0		81	-44	0	
13	80	-40	10; 21; 5		81	-42	10; 23; 7	
	S-Cd-S (same ligand)	***S-Cd-S-C (same ligand)***			***S-Cd-S (same ligand)***	***S-Cd-S-C (same ligand)***		
14	71	128			71	128		
15	71	131			71	131		
16	71	130			71	130		
	N-Cd-N	***N-Cd-N-N (same ligand)***	***N-Cd-N-N***	***Cd-N-N-B***	***N-Cd-N***	***N-Cd-N-N (same ligand)***	***N-Cd-N-N***	***Cd-N-N-B***
17	112; 92	29;30	-111; 29; 94; 145; -30; -149; 94; -110; 29; -150; 146; -30;	-12; 14	112; 92	25	-113; 25; 98; 142; -25; -146; 99; -114; 26; -145; 142; -26	-17; 16; -15
	S-Cd-N	***N-Cd-N-N (same ligand)***	***S-Cd-N-N***	***S'-Cd-N-N***	***S-Cd-S***	***N-Cd-N-N (same ligand)***	***S-Cd-N-N***	***S'-Cd-N-N***
18	69	37;-44; -46	-46; 46; 44; -37; 37; -44	180; 145; -146	68	-37; 44; -44	-43; 47; 43; -37; 39; -44	176;143; -145
19	70	-51; -53;-30	-180; 129; -131	174; -159; 156	70	-53; 51;-29	171; 129; -132	-179; -157; 153
	O-Cd-O	***N-Cd-N-N (same ligand)***	***O-Cd-N-N***	***O'-Cd-N-N***	***O-Cd-O***	***N-Cd-N-N (same ligand)***	***O-Cd-N-N***	***O'-Cd-N-N***
20	82	-14; 61; -35	-153; 166; -159	121; 76; -108;	82	-18; 67; 28; -25; -60; 56	-133; 152; -140	136; -118
21	84	-26; 53; 30; -39; -52; 53	-148; 153; -168	126; -121; 35;	85	-22; 54; 28; -41; -52; 57;	-148; 155; -176	123; -118; 7
22	83	-52; 44; 55; -36; 35; -35;	-130; 138; -148	-130; 129; 147	83	-51; 58; 46; -24; 29; -49;	-154; -96; 159;	61; -61; -142
23	80	-29; 50; 35; -43; -48; 54	-153; 156; -162	128;-124; -18	80	-27; 49; 33; -45; -49; 2	-154; 157; -163	128; -122; -13
24	57	-48; 43; 48; -43; -41;41	-159; -160; 148;	159; -148; 160	56	-47; 43; -47; 43; -42; 42;	-159; -159; 148	160; -148; 159
	O-Cd-O_{ax}	***O-Cd-O-C (same lilngad)***	***O-Cd-O-C***		***O-Cd-O_{ax}***	***O-Cd-O-C (same lilngad)***	***O-Cd-O-C***	
25	180	-32; 29; -29; 32	-107;-148; -102; 11		180	24; -24; -25; 24	-86; -156; -104; 155	
26	175	33; -27; 30; -29	149;-35; -109;-151		176	22;-23; 33; -30	155; 88; -146; 37	

Coordinates of the 20 snapshots obtained from MD simulatio

Snapshot 1

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O	3.626083	0.985525	2.357416
O	5.390150	-0.151843	0.859897
O	1.586494	-0.373843	1.512748
Cd	0.025060	0.184701	-0.038295
O	-1.967493	1.032205	-0.969010
O	-1.445252	-0.213500	1.582293
O	0.614407	2.450871	-0.389238
O	1.414305	0.029021	-2.057501
O	-0.941487	-2.135535	-0.791287
O	1.287871	-2.384134	-2.452382
O	0.501961	3.465931	-2.689385
O	3.243383	-2.236192	1.147055
O	2.271411	-4.632966	1.160642
O	0.402211	-5.964217	0.548307
O	-4.389510	1.303261	-0.094956
O	-4.271471	2.173183	2.315446
O	2.711201	-4.548338	-2.187865
O	3.817606	-4.200262	-4.478200
O	1.796716	-2.786781	-5.264023
O	1.647088	-6.886728	-1.731171
O	-2.548515	-2.401781	2.496573
Cl	-3.030305	-3.419254	1.486279
O	-3.916455	-4.518072	2.093278
O	-1.756965	-4.117715	1.019592
O	-3.725292	-2.781329	0.387218
O	-1.625643	-6.405407	-1.054697
O	-3.147075	-7.110869	0.728761
O	4.048694	1.101073	4.952992
O	4.815826	-3.030767	-0.811854
O	5.224239	-2.202690	-3.212352
O	-0.512012	-7.714286	-3.052749
O	-0.624459	-6.699227	-5.352895
O	-0.499224	3.759751	1.608814
O	-2.020657	3.054288	3.392272
O	-1.685572	1.971324	5.423248
O	1.528631	4.200940	3.211818
O	3.397830	5.532191	3.824154
O	0.280161	1.345548	-4.256209
O	-0.346250	0.388319	-6.442869
O	0.576833	-7.245346	2.857733
O	1.517199	-5.115344	3.803090
O	3.916957	-5.591510	4.512938
O	1.703252	2.919810	5.521244
O	2.643617	5.049813	6.466601
O	0.976290	5.790538	-3.869076
O	-0.150129	-4.374620	-6.532586
O	-2.173603	-3.582435	-7.427293
O	-2.958506	-1.429304	-6.162496
O	2.773507	3.278430	0.932340
O	3.837620	5.616820	0.475646
O	4.944024	5.964895	-1.814688
O	2.923134	7.378377	-2.600510
O	2.414289	7.781023	0.211129
O	-5.029122	4.592419	3.139644
O	-0.472556	-3.475275	4.487720
O	-5.628793	2.676697	-2.024787

O	**-4.430073**	**2.822377**	**-4.213743**
O	**-3.302197**	**5.222786**	**-4.148211**
O	**-5.185364**	**6.622162**	**-4.014312**
O	**-2.373818**	**4.291503**	**-1.881730**
O	**-2.430133**	**5.793210**	**0.280101**
O	**-0.005588**	**-0.543366**	**3.824298**
O	**-2.543405**	**1.002629**	**-3.618571**
O	**-5.218352**	**6.401193**	**1.156486**
O	**4.823511**	**-1.396046**	**5.733978**
O	**3.268259**	**-3.066233**	**7.216008**
O	**4.780155**	**-3.203691**	**3.508379**
O	**-5.890848**	**4.010975**	**5.682300**
O	**-3.867375**	**3.218790**	**6.577005**
O	**-4.341704**	**0.894181**	**7.756695**
O	**-4.563501**	**-1.226203**	**6.189871**
O	**-5.189912**	**-2.183430**	**4.003210**
O	**-3.622562**	**-1.372926**	**-2.757504**
O	**-5.974489**	**-0.828746**	**-3.743169**
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O	**4.283953**	**2.839679**	**-3.165307**
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O	**6.174102**	**1.250969**	**-2.468764**
O	**4.163924**	**0.439363**	**-3.770453**
O	**4.371107**	**-0.903527**	**-5.958362**
O	**8.111926**	**-0.494485**	**-3.230074**
O	**-7.332480**	**4.877109**	**-2.052371**
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Snapshot 2

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Snapshot 3

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Snapshot 4
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Snapshot 5

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Snapshot 6

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Snapshot 7

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Snapshot 8

305

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Snapshot 9

305			
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H	**3.905835**	**4.542890**	**-5.417262**
H	**2.599275**	**-4.888941**	**6.628791**
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H	**1.270860**	**-7.178553**	**-2.363334**
H	**4.671871**	**-2.638734**	**4.932345**
H	**4.234488**	**-1.147414**	**4.754881**
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H	**0.455430**	**5.631949**	**6.346652**
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H	**4.332593**	**4.662996**	**1.271008**
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H	**6.857337**	**0.568948**	**-0.657750**
H	**8.253779**	**-0.004983**	**0.037544**
H	**3.177468**	**3.762654**	**-0.673381**
H	**3.835519**	**5.025560**	**-1.500088**
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H	**4.038390**	**-5.042955**	**4.405734**
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H	**6.529544**	**-3.099056**	**1.609713**
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Snapshot 11

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O	**-5.459305**	**-3.228131**	**2.263892**
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Snapshot 12

284

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H	-4.344828	5.759193	-4.249941
H	-4.704105	5.286516	-1.092221
H	-4.383882	4.673049	-2.458286
H	-0.057695	5.762463	6.084779
H	-0.694805	4.352575	6.170967
H	-3.749245	3.181763	4.827777
H	-3.449650	2.282449	6.074008
H	-0.259214	3.930535	4.152896
H	-0.813395	2.481465	4.471626
H	-3.953563	-0.876808	6.961292
H	-4.981637	-2.153827	6.892331
H	-2.869972	-3.257742	7.793771
H	-1.246706	-3.337690	7.394997
H	-7.778993	4.206909	3.138095
H	-7.585082	3.029741	4.205108

Snapshot 13

287			
O	2.878477	-2.632785	2.181665
O	2.557051	-2.496026	4.694945
O	0.453525	-1.676667	1.408000
Cd	-0.019878	0.116621	-0.068804
O	-0.645007	2.170686	-1.118393
O	-1.105502	1.122951	1.773155
O	2.016439	1.289493	0.513777
O	1.053622	-0.432698	-2.186447
O	-1.789042	-1.131967	-0.984733
O	-3.999379	0.193604	-0.970813
Cl	-4.722726	0.039110	0.359416
O	-5.929840	-0.814359	0.277545
O	-3.764006	-0.462430	1.506166
O	-5.070711	1.492459	0.707488
O	-0.339068	-3.953203	0.437360
O	-2.672831	-4.204714	-0.759039
O	-4.678511	-3.151588	-1.851975
O	1.925941	3.265232	2.270034
O	3.331060	1.629403	3.837171
O	5.336741	0.576277	4.930106
O	-6.083630	-1.515759	-3.419111
O	-5.993133	-3.491498	-5.175368
O	2.643004	2.190876	-1.916687
O	-1.168175	2.050136	-3.767993
O	1.321275	1.638718	-4.211895
O	0.815162	2.437332	-6.459064
O	-1.614148	2.497457	-7.217713
O	-2.698239	0.886207	-5.508820
O	-1.766389	4.674187	-3.873456
O	-3.979445	5.522521	-3.771581
O	-0.782339	5.510329	-1.634508
O	-4.072250	4.223384	-1.514702

O	1.774594	4.824558	-1.454927
O	2.909192	6.353600	-3.033970
O	2.520854	5.705559	0.914521
O	1.984490	0.059233	5.592201
O	3.812201	0.741999	7.183618
O	-6.025082	-4.721757	-0.096943
O	-4.197370	-4.038993	1.494473
O	-7.984490	-1.067131	-1.528013
O	-8.460341	-2.870190	-0.450398
O	-0.918050	-2.009240	-3.415879
O	-1.021299	-1.412177	-5.944842
O	-0.985881	-4.668758	-3.694162
O	0.840720	-4.664368	-5.442480
O	1.817167	-2.740985	-6.169452
O	-0.636754	-6.711303	-1.927830
O	-0.165931	-5.818588	2.435030
O	0.641659	-5.067221	4.929714
O	-1.633433	-4.928885	6.174614
O	-3.771125	-3.450720	6.120522
O	4.041898	-0.139044	1.841130
O	-3.967674	-4.920036	-3.848014
O	-4.702443	-2.193773	3.494818
O	-5.678890	-4.117157	4.221792
O	2.748483	-3.997930	-3.543750
O	4.886176	-5.476094	-3.489658
O	3.907997	-1.544291	-3.433171
Cl	4.591445	-1.450377	-2.052133
O	3.415181	-1.656451	-1.008965
O	5.667563	-2.547755	-1.879595
O	5.208467	-0.085372	-1.916000
O	5.034735	-1.622972	-5.948276
O	2.202411	-4.439410	-0.864007
O	1.998939	-7.002465	-1.030125
O	1.906133	-8.301601	1.226753
O	4.702799	-4.339073	0.232968
O	-6.104499	2.532242	-2.355915
O	-2.887173	-6.401799	2.450290
O	-3.252180	-7.405511	0.827548
O	5.233369	2.950899	-2.630817
O	5.649422	5.003595	-3.555549
O	6.068839	1.363592	-4.425526
O	8.278499	-1.753548	-1.247091
O	8.850290	0.116625	0.246663
O	7.023688	0.112234	1.994981
O	7.091519	2.771752	2.273265
O	6.988270	3.368815	-0.255698
O	7.372817	-1.930311	3.761314
O	6.372327	-4.011138	2.972271
O	6.220528	3.649025	4.704411
O	-2.158246	3.855407	0.559636
O	-1.917001	4.769439	3.013164
O	-4.275808	5.326097	3.911289
O	-8.879759	0.769813	0.419578
O	-5.704447	2.984542	3.205208
O	-5.198334	2.185926	5.452378
O	-8.133756	3.044665	2.446559
O	2.243801	4.778887	-5.752984
O	-5.488717	0.924567	-4.774624
O	-1.275585	8.185912	-2.508487
O	5.196045	-7.014657	1.106947

O	**4.757391**	**-2.624519**	**6.516692**
O	**-0.681419**	**7.066390**	**4.190048**
O	**-0.870188**	**5.550803**	**6.108724**
O	**-1.286240**	**3.498107**	**7.033456**
O	**-0.450770**	**1.910799**	**5.238747**
O	**1.905072**	**7.313233**	**3.333229**
O	**5.311330**	**5.667198**	**0.180325**
O	**-1.484874**	**-1.075761**	**3.715995**
O	**-7.540908**	**-0.864966**	**3.719430**
O	**0.393943**	**8.513850**	**0.230818**
O	**-6.144316**	**6.706397**	**-0.306425**
H	**2.780229**	**-2.734414**	**3.264000**
H	**3.146988**	**-3.376727**	**1.658758**
H	**0.440865**	**9.106480**	**1.039414**
H	**-0.438441**	**8.757849**	**-0.350693**
H	**-0.185480**	**-5.180012**	**1.634024**
H	**-1.181114**	**-6.025334**	**2.510227**
H	**2.187164**	**-3.978182**	**-1.759337**
H	**3.046599**	**-4.350510**	**-0.499623**
H	**5.168394**	**-3.864433**	**-0.465116**
H	**5.191013**	**-5.234864**	**0.377013**
H	**-1.286940**	**3.014500**	**-3.960372**
H	**-0.192857**	**1.829598**	**-4.002632**
H	**7.392540**	**-1.978412**	**-1.685612**
H	**8.428688**	**-2.582318**	**-0.616335**
H	**-3.187022**	**-5.002657**	**-0.803749**
H	**-3.211970**	**-3.437065**	**-1.193926**
H	**-2.115934**	**1.352666**	**-4.790972**
H	**-2.307572**	**0.018075**	**-5.450168**
H	**1.312336**	**2.113398**	**-5.160150**
H	**1.664427**	**0.766598**	**-4.471779**
H	**6.298041**	**2.139810**	**-5.023471**
H	**5.519444**	**0.744737**	**-5.012784**
H	**-3.039006**	**4.226751**	**0.286512**
H	**-2.015812**	**4.271121**	**1.511211**
H	**-1.156215**	**-4.096533**	**-0.138154**
H	**0.525684**	**-4.025931**	**-0.065599**
H	**-8.702835**	**1.336666**	**-0.437552**
H	**-8.416192**	**1.400609**	**1.085676**
H	**-5.924612**	**0.630541**	**-5.650966**
H	**-4.523683**	**0.971492**	**-4.960420**
H	**-2.721441**	**5.096652**	**3.463778**
H	**-1.333393**	**4.184971**	**3.539777**
H	**3.630026**	**2.425397**	**-2.108908**
H	**2.208142**	**2.125629**	**-2.792440**
H	**-5.281847**	**2.513828**	**2.431691**
H	**-6.623330**	**2.738716**	**3.006180**
H	**-1.633619**	**-1.551165**	**4.540738**
H	**-0.762040**	**-1.527992**	**3.260222**
H	**-1.529096**	**-1.464336**	**-6.774451**
H	**-0.066973**	**-1.411834**	**-6.214808**
H	**2.925388**	**-3.063655**	**-3.704882**
H	**2.123694**	**-4.333064**	**-4.253397**
H	**0.335698**	**7.076836**	**3.942856**
H	**-1.154002**	**6.384886**	**3.659664**
H	**0.247815**	**-6.887563**	**-1.549075**
H	**-1.275696**	**-6.798277**	**-1.179173**
H	**-3.532826**	**-5.644611**	**2.332225**
H	**-3.130259**	**-6.917413**	**3.330025**
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H	**-0.246082**	**-4.624830**	**-4.375217**
H	**3.315373**	**-2.451721**	**5.290180**
H	**2.289177**	**-1.542599**	**4.664436**
H	**-1.136327**	**-1.639193**	**-4.343986**
H	**-0.979289**	**-3.049703**	**-3.401974**
H	**2.096748**	**4.209183**	**1.937491**
H	**1.931677**	**2.642180**	**1.511532**
H	**-4.875579**	**-4.219153**	**0.781384**
H	**-3.399994**	**-3.694939**	**1.067632**
H	**2.361825**	**0.645267**	**4.890898**
H	**1.018008**	**0.411073**	**5.642929**
H	**-4.370802**	**-1.413535**	**3.024846**
H	**-4.589708**	**-2.831307**	**2.661108**
H	**0.196259**	**5.107223**	**-1.649064**
H	**-1.242742**	**5.155710**	**-0.843718**
H	**3.985511**	**-4.987084**	**-3.550440**
H	**5.595137**	**-5.167270**	**-4.066896**
H	**-2.164695**	**3.355960**	**-7.183592**
H	**-2.137568**	**1.954562**	**-6.563322**
H	**2.885431**	**-7.294487**	**-1.437418**
H	**2.103668**	**-6.004255**	**-0.959799**
H	**2.549288**	**6.093424**	**-3.900476**
H	**3.848486**	**6.090941**	**-3.101860**
H	**1.004751**	**-4.169931**	**4.786254**
H	**0.412975**	**-5.396796**	**4.012891**
H	**0.605358**	**-5.312065**	**-6.242886**
H	**1.247227**	**-3.859370**	**-5.930196**
H	**-5.406364**	**3.064335**	**-1.883931**
H	**-5.728241**	**2.006046**	**-3.072052**
H	**3.934196**	**-1.005810**	**1.398838**
H	**5.015095**	**0.011709**	**1.834694**
H	**-1.393569**	**4.996407**	**-2.942590**
H	**-1.541924**	**5.416840**	**-4.563910**
H	**3.496378**	**0.933141**	**3.187467**
H	**3.033576**	**2.454875**	**3.385760**
H	**1.237335**	**-7.822776**	**1.707806**
H	**2.001641**	**-7.694132**	**0.453509**
H	**-4.896966**	**6.065516**	**3.648658**
H	**-4.819238**	**4.441032**	**3.954324**
H	**0.546921**	**-1.045637**	**-2.803272**
H	**-1.174031**	**2.900939**	**-0.608157**
H	**-2.687168**	**-0.666526**	**-0.936469**
H	**-0.167949**	**-2.429635**	**1.070308**
H	**2.406572**	**1.534082**	**-0.426277**
H	**-1.738890**	**0.479385**	**2.265905**
H	**2.728302**	**0.785466**	**0.904132**
H	**-1.580289**	**1.802024**	**1.327573**
H	**-1.136407**	**2.041555**	**-1.980230**
H	**-1.640673**	**-1.410522**	**-1.944924**
H	**1.923555**	**-0.824482**	**-1.948607**
H	**1.351301**	**-2.107006**	**1.731058**
H	**5.826346**	**5.570447**	**-4.412679**
H	**6.112989**	**5.634391**	**-2.889451**
H	**1.237762**	**1.966618**	**-7.232580**
H	**-0.103721**	**2.191507**	**-6.658092**
H	**4.885991**	**-2.098376**	**-5.123534**
H	**5.757569**	**-2.075202**	**-6.404049**
H	**2.148809**	**-1.960746**	**-6.639426**
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H	**1.622643**	**5.518306**	**-6.015615**

H	**1.700371**	**3.893822**	**-5.709949**
H	**4.782984**	**-2.492919**	**7.492647**
H	**4.914827**	**-3.554778**	**6.452646**
H	**6.419248**	**-3.418507**	**3.780869**
H	**5.539942**	**-3.767137**	**2.390762**
H	**-3.226587**	**-7.273911**	**1.803503**
H	**-3.094744**	**-8.335770**	**0.763502**
H	**6.174643**	**-7.417764**	**1.092392**
H	**4.735642**	**-7.369276**	**1.897738**
H	**4.822548**	**-0.221666**	**4.885395**
H	**4.797602**	**1.343927**	**4.495219**
H	**5.893635**	**6.133658**	**0.898172**
H	**5.701998**	**4.799068**	**0.238975**
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H	**-0.406620**	**6.181599**	**6.774822**
H	**2.084960**	**5.411533**	**0.038178**
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H	**1.990838**	**3.832787**	**-1.675948**
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H	**8.257386**	**-2.106571**	**4.140069**
H	**6.733875**	**-2.017286**	**4.509971**
H	**7.323382**	**-0.513101**	**2.689295**
H	**7.763487**	**0.156162**	**1.313926**
H	**6.873243**	**3.141798**	**1.345160**
H	**7.030280**	**1.731288**	**2.287169**
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H	**3.133991**	**0.561837**	**6.470530**
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H	**8.614927**	**-0.531073**	**-0.553742**
H	**9.256797**	**0.921623**	**-0.241052**
H	**2.603206**	**7.845326**	**3.805214**
H	**2.281330**	**6.787037**	**2.617093**
H	**5.322401**	**4.114464**	**4.752675**
H	**6.368895**	**3.370469**	**3.744220**
H	**-7.643618**	**-0.532526**	**-0.784108**
H	**-7.209442**	**-1.128836**	**-2.207033**
H	**-5.912823**	**-0.571809**	**-3.751654**
H	**-6.077893**	**-2.138812**	**-4.177612**
H	**-5.647746**	**-4.135724**	**-0.798247**
H	**-6.991563**	**-4.369917**	**-0.046216**
H	**-4.075376**	**-5.786801**	**-4.290308**
H	**-2.994477**	**-4.769283**	**-3.854451**
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H	**-6.163865**	**7.344972**	**-1.107431**
H	**-7.159498**	**6.499651**	**-0.231228**
H	**-0.809991**	**8.660552**	**-3.206572**
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H	**-3.092954**	**5.230499**	**-4.178873**
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H	-4.395915	-3.785854	5.410874
H	-2.534098	-4.439874	6.113833
H	-0.924472	-4.620060	5.597375
H	-8.684303	3.903168	2.480681
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H	-5.914252	-4.764854	3.421387
H	-5.272382	-3.312160	3.734076
H	-8.231139	-2.093974	-1.048343
H	-9.009735	-3.489046	-1.037657

Snapshot 14

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O	3.083333	1.746539	-2.700952
O	2.446795	1.514823	-5.260558
O	3.868085	3.751965	-1.153949
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O	0.070805	3.184994	-1.313678
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O	3.105074	1.654558	0.894205
Cl	4.121555	1.974759	2.025178
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O	3.294535	2.298934	3.330370
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O	6.137155	-1.963720	-4.686784
O	2.504625	-3.474090	-1.470976
O	0.505931	-4.332060	-2.945516
O	-0.338173	-3.194842	-4.724447
O	-0.456808	-5.119835	-6.295537
O	-0.391810	-6.531124	-5.016883
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299
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O	**2.237317**	**-6.979772**	**-4.136299**
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O	**-2.687955**	**7.007707**	**-0.958515**
O	**-3.434634**	**7.506321**	**1.431017**
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O	**0.908757**	**-2.533537**	**-5.303048**
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Snapshot 18

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Snapshot 19

302			
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Snapshot 20

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H	**-0.496502**	**4.300991**	**-4.725208**
H	**-0.840360**	**3.757368**	**5.563727**
H	**0.217255**	**2.612148**	**5.380143**
H	**0.967870**	**1.452859**	**-3.891646**
H	**0.782172**	**3.043761**	**-3.356221**
H	**-1.868717**	**-4.215551**	**2.273283**
H	**-1.503448**	**-2.759053**	**1.742449**
H	**4.263199**	**4.031054**	**1.630525**
H	**3.583024**	**4.288024**	**0.242314**
H	**-0.286667**	**0.384510**	**5.323607**
H	**1.250839**	**-0.017892**	**5.592655**
H	**5.118013**	**0.599017**	**0.570846**
H	**4.627681**	**2.044393**	**1.043373**
H	**-1.349582**	**-6.004464**	**-1.602096**
H	**0.227426**	**-5.531835**	**-1.273885**
H	**-4.309794**	**4.952815**	**-3.302378**
H	**-5.834666**	**5.657505**	**-3.382785**
H	**-0.452207**	**-3.369503**	**-7.729848**
H	**-0.151521**	**-2.139298**	**-6.670140**
H	**-2.647458**	**7.540165**	**-1.499763**
H	**-1.698733**	**6.245298**	**-1.402851**
H	**-4.102092**	**-6.249425**	**-3.490514**
H	**-5.214138**	**-6.387171**	**-2.448847**
H	**0.818373**	**4.744810**	**4.675111**
H	**0.926628**	**5.956703**	**3.474415**

H	**-2.139312**	**4.401513**	**-6.275783**
H	**-1.396697**	**2.965360**	**-6.056505**
H	**4.608291**	**-2.508834**	**-3.223965**
H	**4.298828**	**-2.102322**	**-4.728996**
H	**-2.820998**	**1.088836**	**2.366164**
H	**-4.139942**	**0.133881**	**2.476621**
H	**-0.179667**	**-5.305819**	**-3.418796**
H	**-0.321981**	**-5.560637**	**-5.027705**
H	**-2.491219**	**-0.683150**	**3.748679**
H	**-1.639905**	**-1.666193**	**4.864511**
H	**-0.137521**	**7.482360**	**1.108713**
H	**-1.139284**	**7.867618**	**-0.092319**
H	**4.957658**	**-5.767253**	**2.362511**
H	**5.124991**	**-4.307965**	**2.898808**
H	**-0.595753**	**1.245912**	**-1.924845**
H	**1.044568**	**-3.029771**	**-0.534196**
H	**2.515462**	**0.119207**	**-1.347420**
H	**0.693853**	**2.489307**	**0.997105**
H	**-2.233850**	**-1.674381**	**-0.152310**
H	**2.273567**	**-1.075669**	**2.222770**
H	**-2.474229**	**-0.843812**	**1.135414**
H	**2.273668**	**-1.636543**	**0.894715**
H	**0.535417**	**-2.298803**	**-1.903044**
H	**1.933928**	**1.521249**	**-1.537443**
H	**-1.989878**	**1.316297**	**-1.209541**
H	**-0.348986**	**1.906564**	**2.050981**
H	**-7.165672**	**-5.239798**	**-3.116930**
H	**-7.090285**	**-5.354737**	**-1.549864**
H	**-3.481910**	**-2.482640**	**-6.822740**
H	**-1.894943**	**-2.595356**	**-6.500659**
H	**-4.749079**	**0.685749**	**-6.140855**
H	**-6.339338**	**1.165340**	**-5.958971**
H	**-8.806477**	**0.395596**	**-3.140199**
H	**-7.268972**	**-0.006807**	**-2.871151**
H	**-3.401797**	**0.610102**	**-7.892959**
H	**-3.892129**	**2.055477**	**-7.420433**
H	**-3.562151**	**-5.756167**	**-6.101297**
H	**-3.394818**	**-4.296879**	**-5.564999**
H	**-2.193833**	**3.969240**	**7.156929**
H	**-2.331340**	**5.396697**	**6.663472**
H	**-6.460342**	**2.914302**	**4.793556**
H	**-4.954493**	**2.988943**	**4.272092**
H	**-5.185355**	**6.534112**	**1.668863**
H	**-3.608346**	**7.006739**	**1.997073**
H	**-4.015439**	**7.232756**	**-0.147838**
H	**-4.157754**	**6.977938**	**-1.756747**
H	**0.105503**	**7.266065**	**-2.620191**
H	**1.611351**	**7.340706**	**-3.141656**
H	**-4.165501**	**1.681159**	**5.938202**
H	**-3.581501**	**0.154070**	**5.489016**
H	**-6.259070**	**-5.048217**	**3.091088**
H	**-6.493906**	**-3.943803**	**1.767940**
H	**1.641937**	**-8.569334**	**3.885971**
H	**1.504431**	**-7.141878**	**3.392515**
H	**1.354137**	**-5.250885**	**5.346876**
H	**1.429525**	**-5.365823**	**6.913942**
H	**-3.279920**	**-5.495355**	**0.719943**
H	**-4.292081**	**-5.199866**	**1.874249**
H	**-7.264696**	**-2.618857**	**-0.277552**
H	**-8.491350**	**-2.949518**	**0.593628**

H	**-3.399209**	**-4.455491**	**-1.268397**
H	**-3.972991**	**-5.855215**	**-1.854188**
H	**-5.183213**	**4.074157**	**5.828143**
H	**-3.747660**	**3.826037**	**5.477210**
H	**-6.298339**	**1.160145**	**3.315955**
H	**-7.062347**	**-0.050771**	**2.688538**
H	**-5.597975**	**-2.898903**	**3.522101**
H	**-5.783672**	**-1.308002**	**4.057526**
H	**-6.480987**	**-3.740825**	**-1.907782**
H	**-6.555331**	**-2.232154**	**-2.437942**
H	**-2.302646**	**-0.320711**	**9.044271**
H	**-2.982821**	**-0.063740**	**7.656060**
H	**-8.705157**	**0.049751**	**1.137964**
H	**-7.962543**	**-1.386403**	**1.357243**
H	**-1.957555**	**-6.860596**	**4.189783**
H	**-2.267018**	**-6.454086**	**2.684752**
H	**-4.050385**	**-4.232555**	**6.066327**
H	**-4.631920**	**-2.830513**	**5.876302**
H	**6.229626**	**0.928110**	**-2.115881**
H	**5.933851**	**1.165337**	**-3.665991**
H	**6.874970**	**-1.649472**	**-3.709603**
H	**8.080571**	**-0.928793**	**-4.276003**
H	**4.697129**	**0.136213**	**-5.140463**
H	**5.062396**	**1.592710**	**-5.671298**
H	**3.744847**	**5.440598**	**-5.047581**
H	**2.425904**	**4.485643**	**-4.937125**
H	**4.074625**	**3.668614**	**-3.665068**
H	**4.925940**	**2.685571**	**-2.549236**
H	**4.331995**	**2.677383**	**-7.566056**
H	**4.091616**	**3.507951**	**-6.278332**
H	**4.646737**	**-7.171706**	**-1.689019**
H	**5.744055**	**-6.133374**	**-1.621659**
H	**-0.000895**	**-9.191826**	**-2.786945**
H	**-0.234315**	**-7.834657**	**-2.099265**
H	**1.188315**	**-4.998411**	**-4.770721**
H	**2.137041**	**-6.293278**	**-4.673809**
H	**4.654144**	**-7.793766**	**1.404153**
H	**4.762399**	**-6.581872**	**0.203457**
H	**3.698251**	**-5.056216**	**-2.162244**
H	**2.696489**	**-4.670958**	**-3.363277**
H	**2.038823**	**-3.751913**	**6.556025**
H	**1.964479**	**-2.243242**	**6.025864**
H	**0.447833**	**1.004732**	**8.000848**
H	**0.204919**	**1.943953**	**9.316876**
H	**5.582852**	**-2.010603**	**4.058519**
H	**5.221396**	**-0.656326**	**4.923939**
H	**0.956833**	**-2.108132**	**4.641907**
H	**2.234608**	**-1.090682**	**4.219700**
H	**7.820960**	**1.721820**	**0.772508**
H	**6.594306**	**1.391158**	**1.643689**
H	**4.948038**	**2.885290**	**5.506618**
H	**5.696423**	**3.632033**	**4.235183**
H	**8.604668**	**0.599850**	**-0.857721**
H	**8.530325**	**2.108521**	**-1.387882**
H	**4.210016**	**4.941729**	**5.161428**
H	**2.685144**	**5.646420**	**5.081020**
H	**8.067603**	**-3.380589**	**0.733960**
H	**8.368287**	**-2.150385**	**1.793667**
H	**6.380497**	**4.390428**	**2.188023**
H	**7.123112**	**2.954273**	**2.407301**

H	**7.013678**	**5.356497**	**0.587101**
H	**6.770764**	**6.295718**	**1.903130**

Calculated δ(^{113}Cd) for the model systems investigated. (1)-(5)[53] (*$CDCl_3$*);(6)-(13)[54] (*$CDCl_3$*);(14)-(16)[55] (*CD_2Cl_2*);(17)-(24)[56] (*$CDCl_3$*);(25)-(26)[57] (*$CDCl_3$*).

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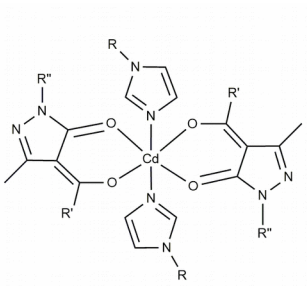
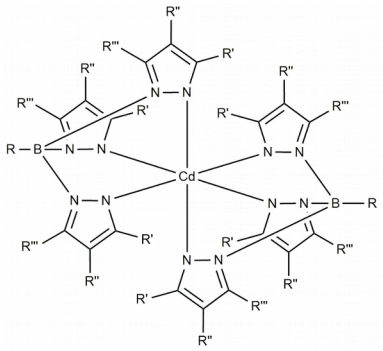
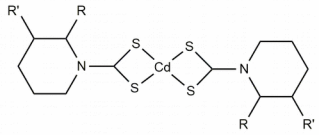


(1) R=Me; R'=R''=Ph
(2) R=Me; R'=Ph; R''=Me
(3) R=$PhCH_2$; R'=R''=Ph
(4) R=$PhCH_2$; R'=Me;R''=Ph
(5) R=$PhCH_2$; R'=Ph; R''=Me

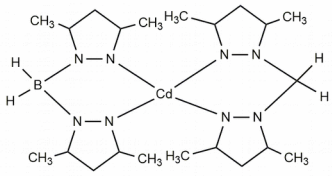


(6) R=R''=R'''=H; R'=Me
(7) R=3-MePz; R'=Me; R''=R'''=H
(8) R=R'=R'''=H; R''=Br
(9) R=R'=R'''=H; R''=Me

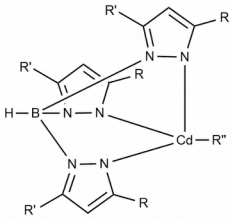
(10) R'=R'''=H; R=4-MePz; R''=Me
(11) R=R''=H; R'=R'''=Me
(12) R=R'=R''=R'''=H
(13) R=Pz; R'=R''=R'''=H



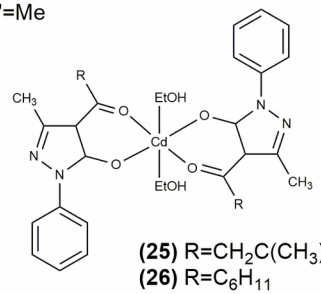
(14) R=R'=H
(15) R=Me; R'=H
(16) R=H; R'=Me



(17)



(18) R=R'=Me; R''=S_2CNEt_2
(19) R=Ph; R'=H; R''=S_2CNEt_2
(20) R=i-Pr; R'=H; R''=$(t\text{-}BuCO)_2CH$
(21) R=Ph; R'=H; R''=$(t\text{-}BuCO)_2CH$
(22) R=Ph; R'=H; R''=$(Ph)_2CH$
(23) R=Ph; R'=H; R''=$(CF_3CO)_2CH$
(24) R=t-Bu; R'=H; R''=CH_3CO_2



(25) R=$CH_2C(CH_3)_3$
(26) R=C_6H_{11}

OP2 geometry [G09; B3LYP/cc-pVDZ_PP (Cd);cc-pVDZ (Light atoms)]

Table S14 Calculated $\delta(^{113}Cd)$, statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31G(d)] level. Data referred wrt 1 M $Cd(ClO_4)_2$. Orange line=ideal correlation

MODEL	Exptl.$\delta(^{113}Cd)$	Calcd $\delta(^{113}Cd)$	ABS diff $\delta(^{113}Cd)$	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	77.10	72.86	4.24	61.76	15.34
2	82.10	84.07	1.97	73.73	8.37
3	76.00	73.70	2.30	62.65	13.35
4	81.20	91.59	10.39	81.77	0.57
5	59.10	73.67	14.57	62.62	3.52
6	200.00	189.35	10.65	186.21	13.79
7	202.50	200.72	1.78	198.35	4.15
8	193.80	197.98	4.18	195.44	1.64
9	195.90	202.38	6.48	200.13	4.23
10	218.30	225.96	7.66	225.32	7.02
11	201.90	200.97	0.93	198.62	3.28
12	198.30	207.28	8.98	205.37	7.07
13	221.10	229.82	8.72	229.45	8.35
14	353.60	340.42	13.18	347.61	5.99
15	365.13	353.09	12.04	361.15	3.98
16	352.13	341.67	10.46	348.94	3.19
17	303.30	298.53	4.77	302.85	0.45
18	265.67	261.82	3.85	263.63	2.04
19	237.50	234.81	2.69	234.79	2.71
20	168.20	173.17	4.97	168.93	0.73
21	172.40	178.93	6.53	175.08	2.68
22	155.20	176.36	21.16	172.34	17.14
23	141.80	152.03	10.23	146.34	4.54
24	148.10	171.63	23.53	167.28	19.18
25	27.20	44.96	17.76	31.94	4.74
26	26.30	34.08	7.78	20.32	5.98

ME	23.53
MAE	8.53
CMAE	6.31
Slope	0.936
Int.	15.06

G09: B3LYP/Sadlej(Cd);6-31G(d)//OP2

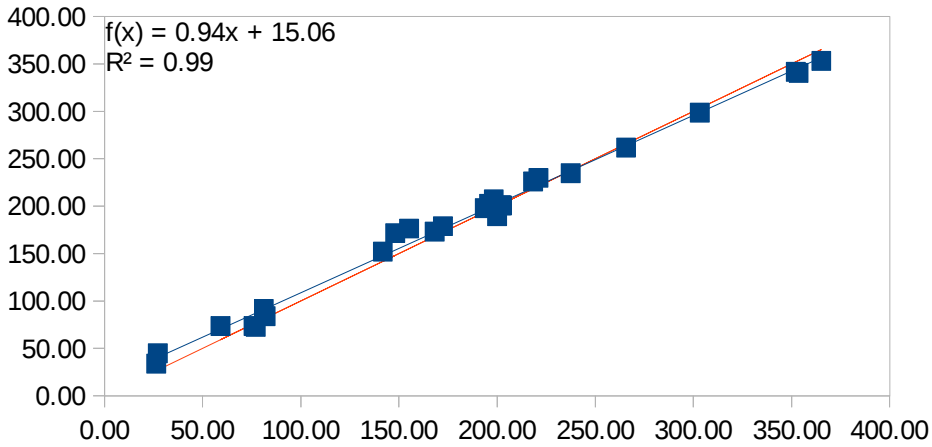


Table S15 Calculated $\delta(^{113}Cd)$, statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31G(d,p)] level. Data referred wrt 1 M $Cd(ClO_4)_2$. Orange line=ideal correlation

MODEL	Exptl.$\delta(^{113}Cd)$	Calcd $\delta(^{113}Cd)$	ABS diff	$\delta(^{113}Cd)$	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	77.10	69.82		7.28	61.11	15.99
2	82.10	81.42		0.68	73.53	8.57
3	76.00	67.39		8.61	58.51	17.50
4	81.20	88.73		7.53	81.35	0.15
5	59.10	76.52		17.42	68.28	9.17
6	200.00	186.61		13.39	186.15	13.86
7	202.50	198.10		4.40	198.45	4.06
8	193.80	194.83		1.03	194.95	1.14
9	195.90	199.09		3.19	199.51	3.60
10	218.30	222.53		4.23	224.60	6.30
11	201.90	198.16		3.74	198.51	3.39
12	198.30	204.02		5.72	204.79	6.48
13	221.10	226.42		5.32	228.77	7.66
14	353.60	337.91		15.69	348.13	5.48
15	365.13	350.52		14.61	361.62	3.51
16	352.13	337.92		14.21	348.14	4.00
17	303.30	296.27		7.03	303.54	0.23
18	265.67	258.97		6.70	263.61	2.07
19	237.50	232.26		5.24	235.01	2.49
20	168.20	170.99		2.79	169.42	1.21
21	172.40	176.59		4.19	175.41	3.01
22	155.20	174.17		18.97	172.83	17.62
23	141.80	149.62		7.82	146.54	4.74
24	148.10	169.81		21.71	168.16	20.05
25	27.20	42.23		15.03	31.57	4.36
26	26.30	31.36		5.06	19.94	6.37
		ME		21.71		
		MAE		8.52		
		CMAE		6.65		
		Slope		0.934		
		Int.		12.74		

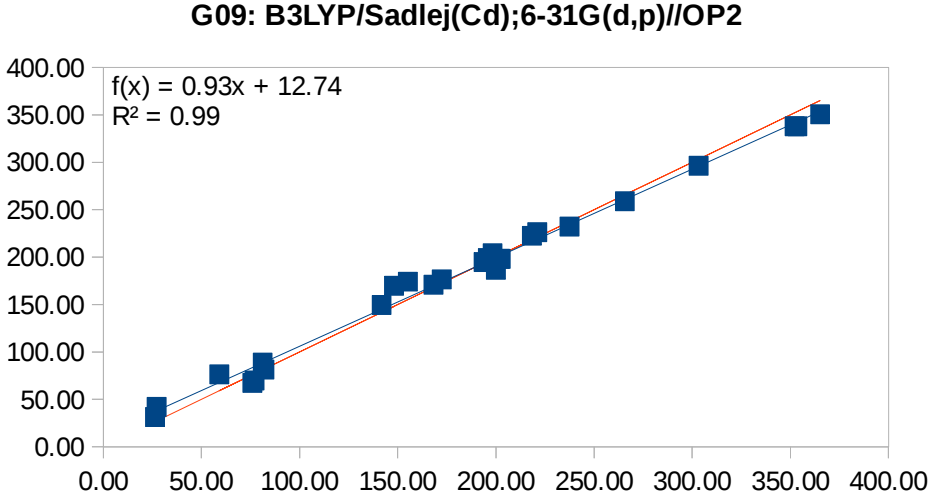


Table S16 Calculated $\delta(^{113}Cd)$, statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31+G(d,p)] level. Data referred wrt 1 M $Cd(ClO_4)_2$. Orange line=ideal correlation

MODEL	Exptl.$\delta(^{113}Cd)$	Calcd $\delta(^{113}Cd)$	ABS diff $\delta(^{113}Cd)$	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	77.10	79.39	2.29	64.22	12.88
2	82.10	87.61	5.51	73.14	8.96
3	76.00	81.45	5.45	66.46	9.54
4	81.20	102.58	21.38	89.39	8.19
5	59.10	76.02	16.92	60.57	1.47
6	200.00	195.59	4.41	190.35	9.65
7	202.50	201.91	0.59	197.20	5.30
8	193.80	200.72	6.92	195.91	2.11
9	195.90	209.63	13.73	205.58	9.68
10	218.30	230.91	12.61	228.67	10.37
11	201.90	205.09	3.19	200.66	1.24
12	198.30	207.13	8.83	202.87	4.57
13	221.10	227.80	6.70	225.30	4.20
14	353.60	335.00	18.60	341.65	11.95
15	365.13	346.78	18.35	354.44	10.69
16	352.13	337.21	14.92	344.05	8.08
17	303.30	303.44	0.14	307.40	4.10
18	265.67	264.84	0.83	265.51	0.16
19	237.50	238.51	1.01	236.93	0.57
20	168.20	175.30	7.10	168.32	0.12
21	172.40	185.37	12.97	179.24	6.84
22	155.20	183.06	27.86	176.74	21.54
23	141.80	159.56	17.76	151.24	9.44
24	148.10	176.95	28.85	170.11	22.01
25	27.20	37.13	9.93	18.36	8.84
26	26.30	29.00	2.70	9.53	16.77
		ME	28.85		
		MAE	10.37		
		CMAE	8.05		
		Slope	0.921		
		Int.	20.22		

G09: B3LYP/Sadlej(Cd);6-31G+(d,p)//OP2

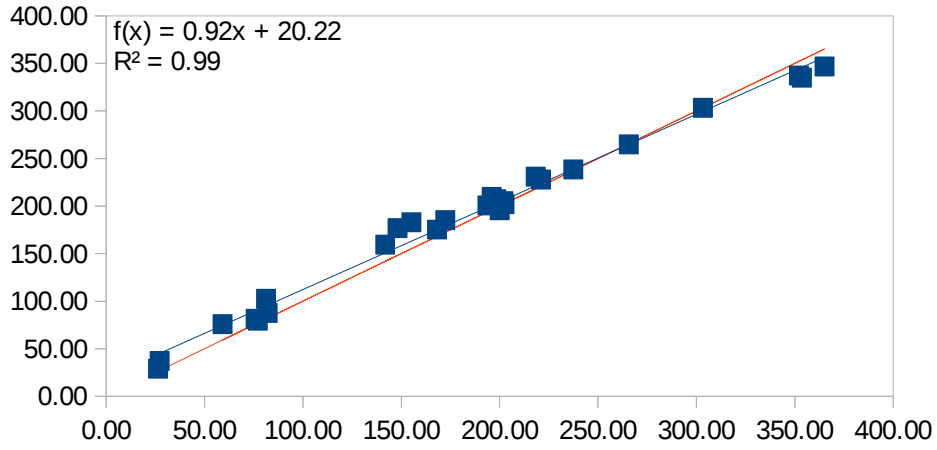


Table S17 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at NR-1 [B3PW91/Sadlej;6-31G(d)]level . Data referred wrt 1 M $Cd(ClO_4)_2$. Orange line=ideal correlation

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	77.10	72.24	4.86	59.82	17.28
2	82.10	83.96	1.86	72.37	9.73
3	76.00	73.20	2.80	60.84	15.16
4	81.20	91.18	9.98	80.10	1.10
5	59.10	73.31	14.21	60.97	1.87
6	200.00	195.97	4.03	192.35	7.65
7	202.50	209.94	7.44	207.32	4.82
8	193.80	201.12	7.32	197.87	4.07
9	195.90	206.24	10.34	203.35	7.45
10	218.30	230.16	11.86	228.98	10.68
11	201.90	208.00	6.10	205.23	3.33
12	198.30	211.12	12.82	208.58	10.28
13	221.10	233.99	12.89	233.08	11.98
14	353.60	334.56	19.04	340.80	12.80
15	365.13	348.60	16.53	355.85	9.28
16	352.13	335.57	16.56	341.88	10.25
17	303.30	299.42	3.88	303.16	0.14
18	265.67	263.10	2.57	264.26	1.41
19	237.50	238.88	1.38	238.32	0.82
20	168.20	174.36	6.16	169.20	1.00
21	172.40	178.00	5.60	173.10	0.70
22	155.20	175.20	20.00	170.10	14.90
23	141.80	149.54	7.74	142.62	0.82
24	148.10	174.49	26.39	169.34	21.24
25	27.20	42.65	15.45	28.12	0.92
26	26.30	31.54	5.24	16.22	10.08
		ME	26.39		
		MAE	9.73		
		CMAE	7.30		
		Slope	0.934		
		Int.	16.40		

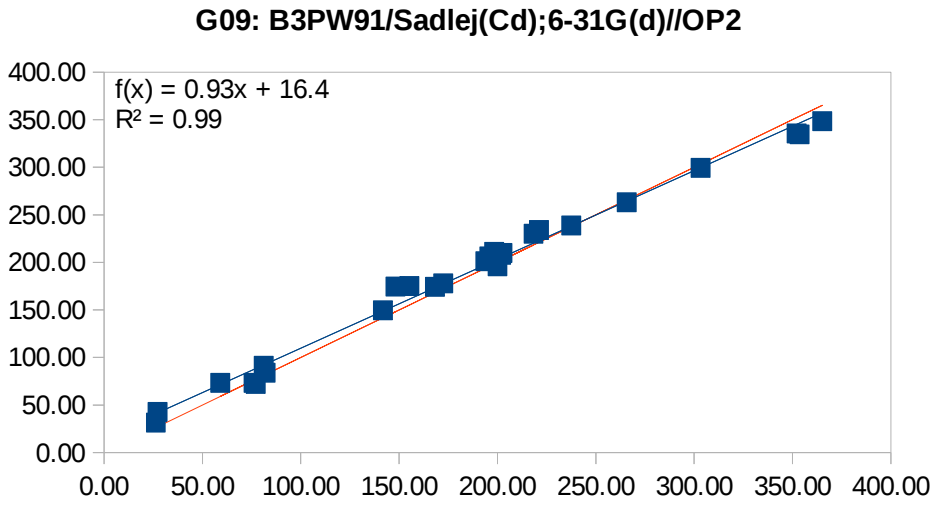


Table S18 Calculated $\delta(^{113}Cd)$, statistical data and graphical correlation obtained at NR-1 [B3PW91/Sadlej;6-31G(d,p)] level. Data referred wrt 1 M $Cd(ClO_4)_2$. Orange line=ideal correlation

MODEL	Exptl.$\delta(^{113}Cd)$	Calcd $\delta(^{113}Cd)$	ABS diff $\delta(^{113}Cd)$	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	77.10	67.34	9.76	60.05	17.05
2	82.10	79.05	3.05	72.59	9.51
3	76.00	68.35	7.65	61.12	14.88
4	81.20	79.31	1.89	72.88	8.32
5	59.10	67.83	8.73	60.56	1.46
6	200.00	191.27	8.73	192.91	7.09
7	202.50	205.45	2.95	208.10	5.60
8	193.80	195.99	2.19	197.96	4.16
9	195.90	200.96	5.06	203.29	7.39
10	218.30	224.76	6.46	228.80	10.50
11	201.90	203.22	1.32	205.72	3.82
12	198.30	205.89	7.59	208.58	10.28
13	221.10	228.64	7.54	232.97	11.87
14	353.60	329.25	24.35	340.82	12.78
15	365.13	339.92	25.21	352.26	12.87
16	352.13	330.08	22.05	341.71	10.42
17	303.30	295.24	8.06	304.36	1.06
18	265.67	258.27	7.40	264.72	0.95
19	237.50	234.37	3.13	239.11	1.61
20	168.20	170.22	2.02	170.33	2.13
21	172.40	173.73	1.33	174.10	1.70
22	155.20	171.08	15.88	171.26	16.06
23	141.80	145.19	3.39	143.50	1.70
24	148.10	170.82	22.72	170.97	22.87
25	27.20	37.94	10.74	28.53	1.33
26	26.30	26.84	0.54	16.63	9.67

ME	25.21
MAE	8.45
CMAE	7.96
Slope	0.933
Int.	11.33

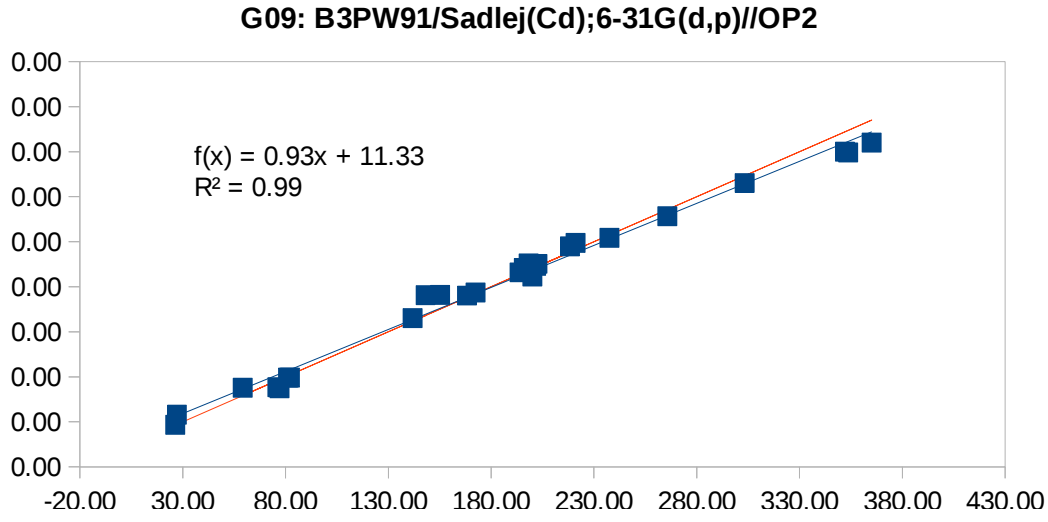


Table S19 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at NR-1 [B3PW91/Sadlej;6-31+G(d,p)] level. Data referred wrt 1 M $Cd(ClO_4)_2$. Orange line=ideal correlation

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	77.10	31.73	45.37	19.43	57.67
2	82.10	42.46	39.64	30.72	51.38
3	76.00	81.69	5.69	71.99	4.01
4	81.20	102.94	21.74	94.35	13.15
5	59.10	76.72	17.62	66.76	7.66
6	200.00	200.97	0.97	197.49	2.51
7	202.50	209.74	7.24	206.72	4.22
8	193.80	203.75	9.95	200.41	6.61
9	195.90	213.60	17.70	210.77	14.87
10	218.30	235.31	17.01	233.62	15.32
11	201.90	210.46	8.56	207.48	5.58
12	198.30	211.20	12.90	208.25	9.95
13	221.10	232.12	11.02	230.27	9.17
14	353.60	329.85	23.75	333.08	20.52
15	365.13	345.10	20.03	349.12	16.01
16	352.13	332.01	20.12	335.36	16.77
17	303.30	303.30	0.00	305.15	1.85
18	265.67	265.79	0.12	265.69	0.02
19	237.50	242.03	4.53	240.68	3.18
20	168.20	182.85	14.65	178.43	10.23
21	172.40	184.96	12.56	180.64	8.24
22	155.20	182.38	27.18	177.94	22.74
23	141.80	157.64	15.84	151.90	10.10
24	148.10	179.97	31.87	175.39	27.29
25	27.20	43.49	16.29	31.81	4.61
26	26.30	32.63	6.33	20.37	5.93
		ME	45.37		
		MAE	15.72		
		CMAE	13.45		
		Slope	0.950		
		Int.	13.26		

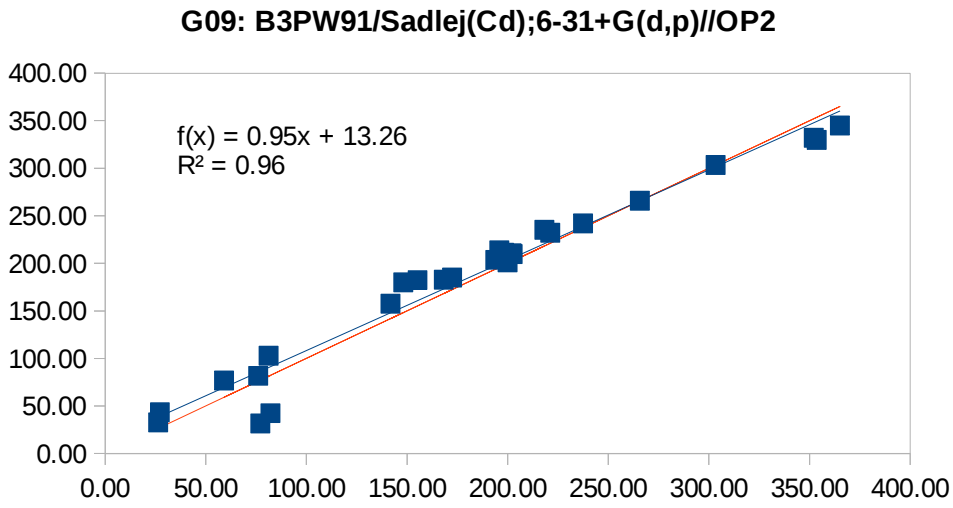


Table S20 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31G(d)]level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	δ(^{113}Cd)$_{fit}$ corrected by fit	ABS diff δ(^{113}Cd)$_{fit}$
1	-629.03	-643.11	14.08	-644.14	15.11
2	-624.03	-631.91	7.88	-632.17	8.14
3	-630.13	-642.28	12.15	-643.25	13.12
4	-624.93	-624.38	0.55	-624.13	0.80
5	-647.03	-642.31	4.72	-643.28	3.75
6	-506.13	-526.63	20.50	-519.70	13.57
7	-503.63	-515.26	11.63	-507.55	3.92
8	-512.33	-517.99	5.66	-510.47	1.86
9	-510.23	-513.60	3.37	-505.77	4.46
10	-487.83	-490.02	2.19	-480.59	7.24
11	-504.23	-515.01	10.78	-507.28	3.05
12	-507.83	-508.69	0.86	-500.54	7.29
13	-485.03	-486.16	1.13	-476.46	8.57
14	-352.53	-375.56	23.03	-358.31	5.78
15	-341.00	-362.88	21.88	-344.77	3.77
16	-354.00	-374.31	20.31	-356.98	2.98
17	-402.83	-417.45	14.62	-403.06	0.23
18	-440.46	-454.16	13.70	-442.28	1.82
19	-468.63	-481.16	12.53	-471.13	2.50
20	-537.93	-542.80	4.87	-536.98	0.95
21	-533.73	-537.05	3.32	-530.83	2.90
22	-550.93	-539.61	11.32	-533.57	17.36
23	-564.33	-563.95	0.38	-559.57	4.76
24	-558.03	-544.35	13.68	-538.63	19.40
25	-678.93	-671.02	7.91	-673.95	4.98
26	-679.83	-681.90	2.07	-685.57	5.74
	ME		23.03		
	MAE		9.43		
	CMAE		6.31		
	Slope		0.936		
	Int.		-40.15		

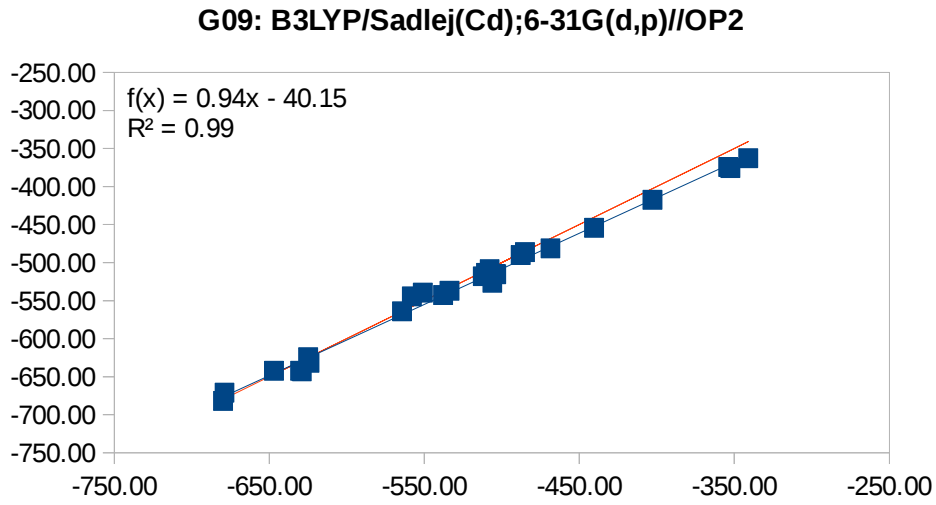


Table S21 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31G(d,p)] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	δ(^{113}Cd)$_{fit}$ corrected by fit	ABS diff δ(^{113}Cd)$_{fit}$
1	**-629.03**	**-639.72**	10.69	-645.00	15.97
2	**-624.03**	**-628.12**	4.09	-632.58	8.55
3	**-630.13**	**-642.15**	12.02	-647.61	17.48
4	**-624.93**	**-620.81**	4.12	-624.76	0.17
5	**-647.03**	**-633.02**	14.01	-637.83	9.20
6	**-506.13**	**-522.93**	16.80	-519.93	13.80
7	**-503.63**	**-511.44**	7.81	-507.62	3.99
8	**-512.33**	**-514.71**	2.38	-511.12	1.21
9	**-510.23**	**-510.45**	0.22	-506.56	3.67
10	**-487.83**	**-487.01**	0.82	-481.46	6.37
11	**-504.23**	**-511.38**	7.15	-507.56	3.33
12	**-507.83**	**-505.52**	2.31	-501.28	6.55
13	**-485.03**	**-483.12**	1.91	-477.29	7.74
14	**-352.53**	**-371.63**	19.10	-357.89	5.36
15	**-341.00**	**-359.02**	18.02	-344.39	3.39
16	**-354.00**	**-371.62**	17.62	-357.88	3.88
17	**-402.83**	**-413.27**	10.44	-402.49	0.34
18	**-440.46**	**-450.57**	10.11	-442.44	1.98
19	**-468.63**	**-477.28**	8.65	-471.05	2.42
20	**-537.93**	**-538.55**	0.62	-536.66	1.27
21	**-533.73**	**-532.95**	0.78	-530.67	3.06
22	**-550.93**	**-535.37**	15.56	-533.25	17.68
23	**-564.33**	**-559.92**	4.41	-559.54	4.79
24	**-558.03**	**-539.73**	18.30	-537.92	20.11
25	**-678.93**	**-667.31**	11.62	-674.56	4.37
26	**-679.83**	**-678.18**	1.65	-686.19	6.36
		ME	19.10		
		MAE	8.51		
		CMAE	6.66		
		Slope	0.934		
		Int.	-37.44		

G09: B3LYP/Sadlej(Cd);6-31G(d,p)//OP2

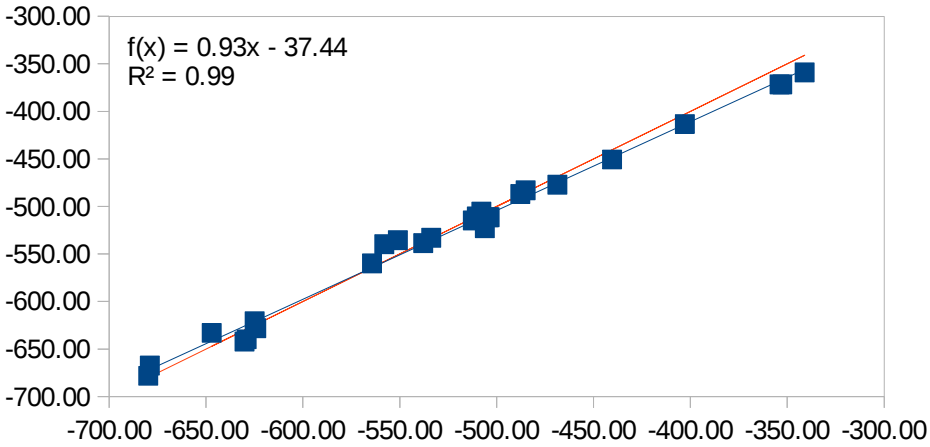


Table S22 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31+G(d,p)] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	δ(^{113}Cd)$_{fit}$ corrected by fit	ABS diff δ(^{113}Cd)$_{fit}$
1	-629.03	-604.82	24.21	-641.91	12.88
2	-624.03	-596.60	27.43	-632.99	8.96
3	-630.13	-602.76	27.37	-639.68	9.55
4	-624.93	-581.63	43.30	-616.74	8.19
5	-647.03	-608.18	38.85	-645.56	1.47
6	-506.13	-488.61	17.52	-515.79	9.66
7	-503.63	-482.29	21.34	-508.93	5.30
8	-512.33	-483.49	28.84	-510.23	2.10
9	-510.23	-474.58	35.65	-500.55	9.68
10	-487.83	-453.30	34.53	-477.46	10.37
11	-504.23	-479.11	25.12	-505.47	1.24
12	-507.83	-477.08	30.75	-503.27	4.56
13	-485.03	-456.41	28.62	-480.83	4.20
14	-352.53	-349.21	3.32	-364.48	11.95
15	-341.00	-337.42	3.58	-351.69	10.69
16	-354.00	-347.00	7.00	-362.08	8.08
17	-402.83	-380.77	22.06	-398.73	4.10
18	-440.46	-419.36	21.10	-440.62	0.16
19	-468.63	-445.69	22.94	-469.20	0.57
20	-537.93	-508.91	29.02	-537.81	0.12
21	-533.73	-498.84	34.89	-526.89	6.84
22	-550.93	-501.15	49.78	-529.39	21.54
23	-564.33	-524.64	39.69	-554.89	9.44
24	-558.03	-507.26	50.77	-536.02	22.01
25	-678.93	-647.08	31.85	-687.78	8.85
26	-679.83	-655.21	24.62	-696.61	16.78
		ME	50.77		
		MAE	27.85		
		CMAE	8.05		
		Slope	0.921		
		Int.	-13.40		

Table S23 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at NR-1 [B3PW91/Sadlej;6-31G(d)] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	-629.03	-623.03	6.00	-646.31	17.28
2	-624.03	-611.31	12.72	-633.76	9.73
3	-630.13	-622.07	8.06	-645.29	15.16
4	-624.93	-604.09	20.84	-626.03	1.10
5	-647.03	-621.96	25.07	-645.16	1.87
6	-506.13	-499.30	6.83	-513.78	7.65
7	-503.63	-485.33	18.30	-498.81	4.82
8	-512.33	-494.15	18.18	-508.26	4.07
9	-510.23	-489.03	21.20	-502.78	7.45
10	-487.83	-465.11	22.72	-477.15	10.68
11	-504.23	-487.27	16.96	-500.90	3.33
12	-507.83	-484.15	23.68	-497.55	10.28
13	-485.03	-461.28	23.75	-473.05	11.98
14	-352.53	-360.71	8.18	-365.33	12.80
15	-341.00	-346.66	5.66	-350.28	9.28
16	-354.00	-359.70	5.70	-364.25	10.25
17	-402.83	-395.85	6.98	-402.97	0.14
18	-440.46	-432.17	8.29	-441.87	1.41
19	-468.63	-456.39	12.24	-467.81	0.82
20	-537.93	-520.91	17.02	-536.93	1.00
21	-533.73	-517.27	16.46	-533.03	0.70
22	-550.93	-520.07	30.86	-536.03	14.90
23	-564.33	-545.73	18.60	-563.51	0.82
24	-558.03	-520.78	37.25	-536.79	21.24
25	-678.93	-652.62	26.31	-678.01	0.92
26	-679.83	-663.73	16.10	-689.91	10.08
		ME	37.25		
		MAE	16.69		
		CMAE	7.30		
		Slope	0.934		
		Int.	-19.65		

Table S24 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at NR-1 [B3PW91/Sadlej;6-31G(d,p)] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	-629.03	-619.64	9.39	-646.08	17.05
2	-624.03	-607.94	16.09	-633.54	9.51
3	-630.13	-618.64	11.49	-645.01	14.88
4	-624.93	-607.67	17.26	-633.25	8.32
5	-647.03	-619.16	27.87	-645.57	1.46
6	-506.13	-495.71	10.42	-513.22	7.09
7	-503.63	-481.53	22.10	-498.03	5.60
8	-512.33	-490.99	21.34	-508.17	4.16
9	-510.23	-486.03	24.20	-502.85	7.38
10	-487.83	-462.22	25.61	-477.33	10.50
11	-504.23	-483.76	20.47	-500.42	3.81
12	-507.83	-481.09	26.74	-497.55	10.28
13	-485.03	-458.34	26.69	-473.16	11.87
14	-352.53	-357.73	5.20	-365.31	12.78
15	-341.00	-347.06	6.06	-353.87	12.87
16	-354.00	-356.90	2.90	-364.42	10.42
17	-402.83	-391.74	11.09	-401.77	1.06
18	-440.46	-428.72	11.74	-441.41	0.95
19	-468.63	-452.61	16.02	-467.02	1.61
20	-537.93	-516.76	21.17	-535.80	2.13
21	-533.73	-513.25	20.48	-532.03	1.70
22	-550.93	-515.90	35.03	-534.87	16.06
23	-564.33	-541.79	22.54	-562.63	1.70
24	-558.03	-516.16	41.87	-535.16	22.87
25	-678.93	-649.04	29.89	-677.60	1.33
26	-679.83	-660.14	19.69	-689.50	9.67
		ME	41.87		
		MAE	19.36		
		CMAE	7.96		
		Slope	0.933		
		Int.	-16.97		

Table S25 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at NR-1 [B3PW91/Sadlej;6-31+G(d,p)] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	δ(^{113}Cd)$_{fit}$ corrected by fit	ABS diff δ(^{113}Cd)$_{fit}$
1	-629.03	-635.97	6.94	-686.70	57.67
2	-624.03	-625.24	1.21	-675.41	51.38
3	-630.13	-586.01	44.12	-634.14	4.01
4	-624.93	-564.75	60.18	-611.78	13.15
5	-647.03	-590.98	56.05	-639.37	7.66
6	-506.13	-466.73	39.40	-508.64	2.51
7	-503.63	-457.95	45.68	-499.41	4.22
8	-512.33	-463.95	48.38	-505.72	6.61
9	-510.23	-454.10	56.13	-495.36	14.87
10	-487.83	-432.39	55.44	-472.51	15.32
11	-504.23	-457.23	47.00	-498.65	5.58
12	-507.83	-456.50	51.33	-497.88	9.95
13	-485.03	-435.57	49.46	-475.86	9.17
14	-352.53	-337.85	14.68	-373.05	20.52
15	-341.00	-322.60	18.40	-357.01	16.01
16	-354.00	-335.68	18.32	-370.77	16.77
17	-402.83	-364.39	38.44	-400.98	1.85
18	-440.46	-401.90	38.56	-440.44	0.02
19	-468.63	-425.67	42.96	-465.45	3.18
20	-537.93	-484.85	53.08	-527.70	10.23
21	-533.73	-482.74	50.99	-525.49	8.24
22	-550.93	-485.31	65.62	-528.19	22.74
23	-564.33	-510.06	54.27	-554.23	10.10
24	-558.03	-487.73	70.30	-530.74	27.29
25	-678.93	-624.20	54.73	-674.32	4.61
26	-679.83	-635.07	44.76	-685.76	5.93
		ME	70.30		
		MAE	43.32		
		CMAE	13.45		
		Slope	0.950		
		Int.	16.725		

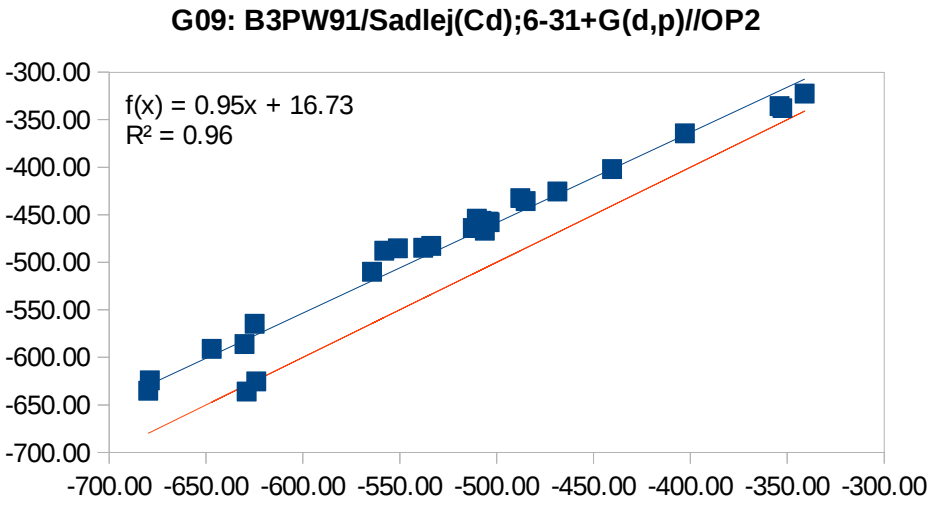


Table S26 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at NR-2 [B3LYP/DZP)] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	-629.03	-707.28	78.25	-636.72	7.69
2	-624.03	-729.03	105.00	-658.29	34.26
3	-630.13	-706.12	75.99	-635.57	5.44
4	-624.93	-695.65	70.72	-625.19	0.26
5	-647.03	-708.80	61.77	-638.23	8.80
6	-506.13	-600.08	93.95	-530.44	24.31
7	-503.63	-578.95	75.32	-509.49	5.86
8	-512.33	-590.60	78.27	-521.04	8.71
9	-510.23	-588.22	77.99	-518.68	8.45
10	-487.83	-556.22	68.39	-486.96	0.87
11	-504.23	-589.60	85.37	-520.05	15.82
12	-507.83	-584.41	76.58	-514.91	7.08
13	-485.03	-557.72	72.69	-488.44	3.41
14	-352.53	-416.33	63.80	-348.26	4.27
15	-341.00	-405.38	64.38	-337.41	3.59
16	-354.00	-416.50	62.50	-348.43	5.57
17	-402.83	-466.55	63.72	-398.05	4.78
18	-440.46	-515.57	75.11	-446.65	6.19
19	-468.63	-532.51	63.88	-463.45	5.18
20	-537.93	-599.43	61.50	-529.80	8.13
21	-533.73	-595.68	61.95	-526.08	7.65
22	-550.93	-599.03	48.10	-529.40	21.53
23	-564.33	-626.52	62.19	-556.65	7.68
24	-558.03	-597.89	39.86	-528.27	29.76
25	-678.93	-734.91	55.98	-664.12	14.81
26	-679.83	-745.89	66.06	-675.00	4.83
		ME	105.00		
		MAE	69.59		
		CMAE	9.81		
		Slope	1.009		
		Int.	-65.06		

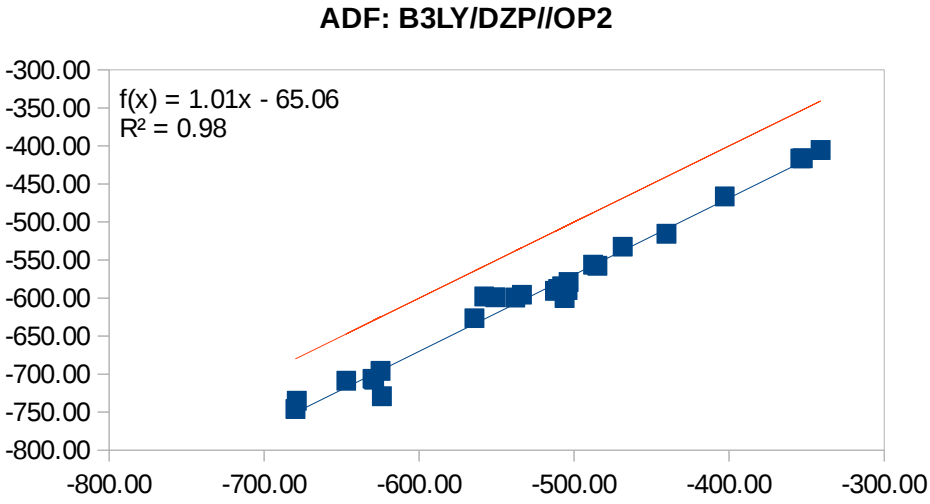


Table S27 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at NR-2 [B3LYP/TZ2P)] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	-629.03	-694.77	65.74	-635.75	6.72
2	-624.03	-715.88	91.85	-656.04	32.01
3	-630.13	-693.26	63.13	-634.29	4.16
4	-624.93	-681.69	56.76	-623.17	1.76
5	-647.03	-695.15	48.12	-636.11	10.92
6	-506.13	-584.51	78.38	-529.73	23.60
7	-503.63	-573.31	69.68	-518.96	15.33
8	-512.33	-581.58	69.25	-526.91	14.58
9	-510.23	-577.55	67.32	-523.03	12.80
10	-487.83	-543.40	55.57	-490.20	2.37
11	-504.23	-568.70	64.47	-514.52	10.29
12	-507.83	-574.19	66.36	-519.80	11.97
13	-485.03	-544.01	58.98	-490.78	5.75
14	-352.53	-397.52	44.99	-349.93	2.60
15	-341.00	-383.02	42.02	-335.99	5.01
16	-354.00	-395.16	41.16	-347.66	6.34
17	-402.83	-448.24	45.41	-398.70	4.13
18	-440.46	-491.90	51.44	-440.68	0.22
19	-468.63	-512.59	43.96	-460.57	8.06
20	-537.93	-582.17	44.24	-527.48	10.45
21	-533.73	-579.81	46.08	-525.21	8.52
22	-550.93	-581.51	30.58	-526.84	24.09
23	-564.33	-610.08	45.75	-554.31	10.02
24	-558.03	-591.27	33.24	-536.23	21.80
25	-678.93	-728.15	49.22	-667.84	11.09
26	-679.83	-737.54	57.71	-676.87	2.96
		ME	91.85		
		MAE	55.05		
		CMAE	10.29		
		Slope	1.040		
		Int.	-33.59		

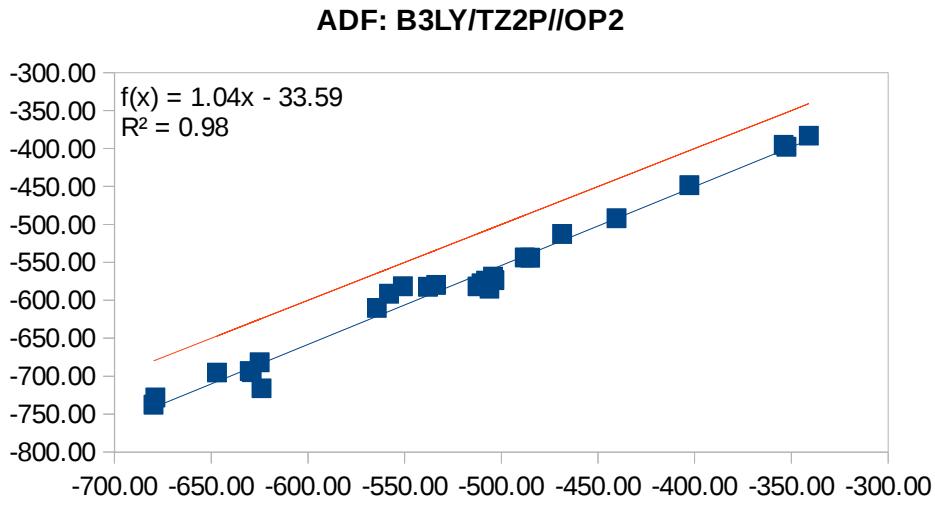


Table S28 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at RS [B3LYP/DZP)] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	-629.03	-667.87	38.84	-632.65	3.62
2	-624.03	-692.02	67.99	-654.99	30.96
3	-630.13	-666.78	36.65	-631.64	1.51
4	-624.93	-648.73	23.80	-614.94	9.99
5	-647.03	-669.19	22.16	-633.87	13.16
6	-506.13	-556.72	50.59	-529.83	23.70
7	-503.63	-546.16	42.53	-520.06	16.43
8	-512.33	-550.21	37.88	-523.80	11.47
9	-510.23	-547.68	37.45	-521.46	11.23
10	-487.83	-518.37	30.54	-494.35	6.52
11	-504.23	-544.15	39.92	-518.20	13.97
12	-507.83	-543.33	35.50	-517.44	9.61
13	-485.03	-515.00	29.97	-491.23	6.20
14	-352.53	-355.26	2.73	-343.46	9.07
15	-341.00	-343.55	2.55	-332.63	8.37
16	-354.00	-354.03	0.03	-342.32	11.68
17	-402.83	-416.50	13.67	-400.11	2.72
18	-440.46	-463.36	22.90	-443.46	3.00
19	-468.63	-487.66	19.03	-465.94	2.69
20	-537.93	-557.57	19.64	-530.61	7.32
21	-533.73	-551.29	17.56	-524.80	8.93
22	-550.93	-555.42	4.49	-528.62	22.31
23	-564.33	-589.34	25.01	-560.00	4.33
24	-558.03	-557.97	0.06	-530.98	27.05
25	-678.93	-703.92	24.99	-666.00	12.93
26	-679.83	-714.93	35.10	-676.18	3.65

ME	67.99
MAE	26.21
CMAE	10.86
Slope	1.081
Int.	16.02

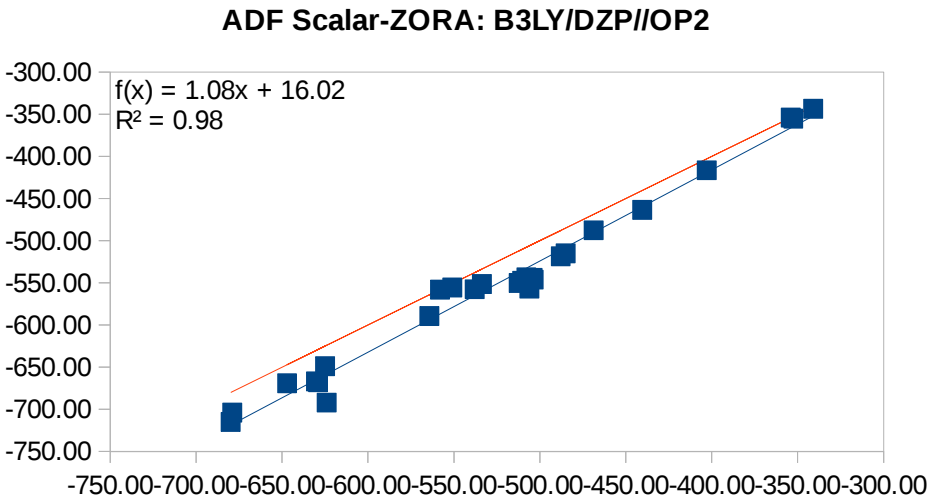


Table S29 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at RS [B3LYP/TZ2P)] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	δ(^{113}Cd)$_{fit}$ corrected by fit	ABS diff δ(^{113}Cd)$_{fit}$
1	-629.03	-682.79	53.76	-626.84	2.19
2	-624.03	-707.43	83.40	-648.09	24.06
3	-630.13	-681.89	51.76	-626.07	4.06
4	-624.93	-670.99	46.06	-616.67	8.26
5	-647.03	-685.34	38.31	-629.04	17.99
6	-506.13	-580.00	73.87	-538.22	32.09
7	-503.63	-564.91	61.28	-525.21	21.58
8	-512.33	-565.03	52.70	-525.32	12.99
9	-510.23	-560.38	50.15	-521.31	11.08
10	-487.83	-532.16	44.33	-496.98	9.15
11	-504.23	-566.13	61.90	-526.26	22.03
12	-507.83	-557.26	49.43	-518.62	10.79
13	-485.03	-529.66	44.63	-494.82	9.79
14	-352.53	-339.45	13.08	-330.83	21.70
15	-341.00	-327.56	13.44	-320.58	20.42
16	-354.00	-339.26	14.74	-330.66	23.34
17	-402.83	-437.22	34.39	-415.12	12.29
18	-440.46	-472.58	32.12	-445.61	5.15
19	-468.63	-495.77	27.14	-465.60	3.03
20	-537.93	-579.50	41.57	-537.79	0.14
21	-533.73	-572.56	38.83	-531.81	1.92
22	-550.93	-573.28	22.35	-532.43	18.50
23	-564.33	-607.07	42.74	-561.56	2.77
24	-558.03	-582.48	24.45	-540.36	17.67
25	-678.93	-721.66	42.73	-660.36	18.57
26	-679.83	-732.18	52.35	-669.43	10.40
		ME	83.40		
		MAE	42.75		
		CMAE	13.15		
		Slope	1.160		
		Int.	44.27		

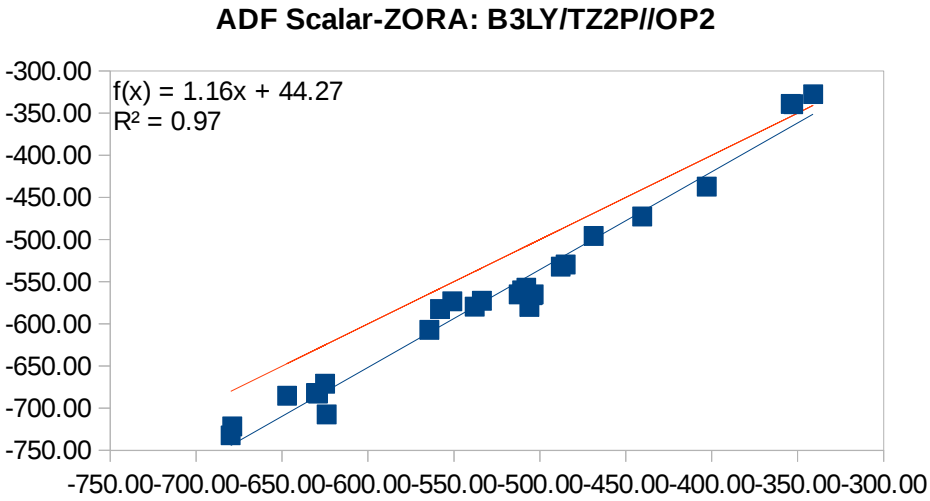


Table S30 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at SO [B3LYP/DZP)] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	-629.03	-701.28	72.3	-635.54	6.51
2	-624.03	-726.12	102.1	-661.24	37.21
3	-630.13	-700.43	70.3	-634.66	4.53
4	-624.93	-683.14	58.2	-616.77	8.16
5	-647.03	-702.56	55.5	-636.86	10.17
6	-506.13	-590.01	83.9	-520.42	14.29
7	-503.63	-586.11	82.5	-516.39	12.76
8	-512.33	-587.68	75.3	-518.01	5.68
9	-510.23	-582.67	72.4	-512.83	2.60
10	-487.83	-554.21	66.4	-483.39	4.44
11	-504.23	-576.77	72.5	-506.73	2.50
12	-507.83	-578.20	70.4	-508.21	0.38
13	-485.03	-550.76	65.7	-479.82	5.21
14	-352.53	-439.08	86.6	-364.28	11.75
15	-341.00	-425.37	84.4	-350.09	9.09
16	-354.00	-438.22	84.2	-363.39	9.39
17	-402.83	-445.91	43.1	-371.34	31.49
18	-440.46	-516.71	76.3	-444.59	4.13
19	-468.63	-549.63	81.0	-478.65	10.02
20	-537.93	-593.37	55.4	-523.90	14.03
21	-533.73	-588.30	54.6	-518.65	15.08
22	-550.93	-592.22	41.3	-522.71	28.22
23	-564.33	-627.63	63.3	-559.34	4.99
24	-558.03	-594.37	36.3	-524.93	33.10
25	-678.93	-744.51	65.6	-680.26	1.33
26	-679.83	-755.83	76.0	-691.98	12.15

ME	102.09
MAE	69.06
CMAE	11.51
Slope	0.967
Int.	-86.98

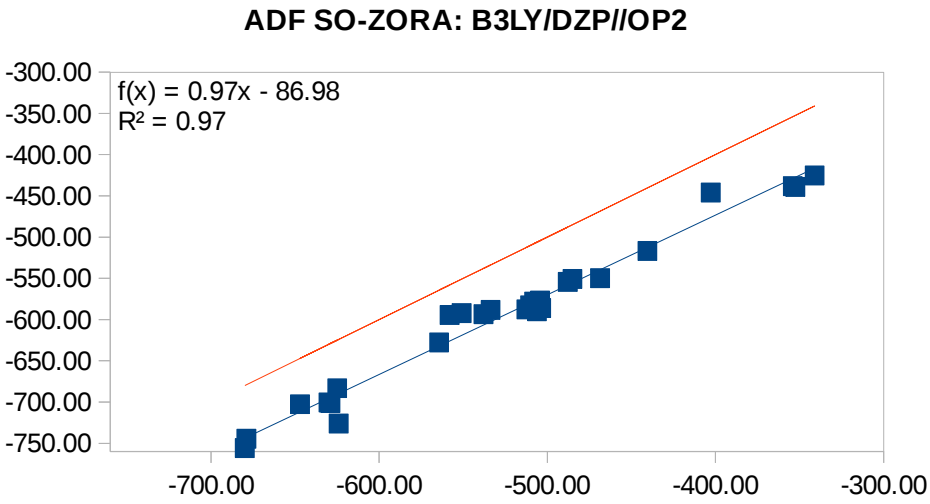


Table S31 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at SO [B3LYP/DZP)] level. Data are given without spin-orbit contributions. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	δ(^{113}Cd)$_{fit}$ corrected by fit	ABS diff δ(^{113}Cd)$_{fit}$
1	-629.03	-668.43	39.40	-632.01	2.98
2	-624.03	-692.74	68.71	-654.28	30.25
3	-630.13	-667.43	37.30	-631.10	0.97
4	-624.93	-649.52	24.59	-614.69	10.24
5	-647.03	-669.74	22.71	-633.21	13.82
6	-506.13	-557.57	51.44	-530.47	24.34
7	-503.63	-549.07	45.44	-522.68	19.05
8	-512.33	-551.57	39.24	-524.97	12.64
9	-510.23	-549.09	38.86	-522.70	12.47
10	-487.83	-519.83	32.00	-495.90	8.07
11	-504.23	-544.74	40.51	-518.71	14.48
12	-507.83	-544.69	36.86	-518.67	10.84
13	-485.03	-516.43	31.40	-492.79	7.76
14	-352.53	-351.74	0.79	-341.93	10.60
15	-341.00	-339.88	1.12	-331.07	9.93
16	-354.00	-351.14	2.86	-341.38	12.62
17	-402.83	-416.36	13.53	-401.12	1.71
18	-440.46	-461.89	21.43	-442.83	2.37
19	-468.63	-487.08	18.45	-465.91	2.72
20	-537.93	-558.38	20.44	-531.21	6.72
21	-533.73	-551.96	18.23	-525.33	8.40
22	-550.93	-556.17	5.24	-529.18	21.75
23	-564.33	-590.89	26.56	-560.99	3.34
24	-558.03	-557.63	0.40	-530.52	27.51
25	-678.93	-705.40	26.47	-665.88	13.05
26	-679.83	-716.45	36.62	-676.00	3.83
		ME	68.71		
		MAE	26.95		
		CMAE	11.25		
		Slope	1.092		
		Int.	21.56		

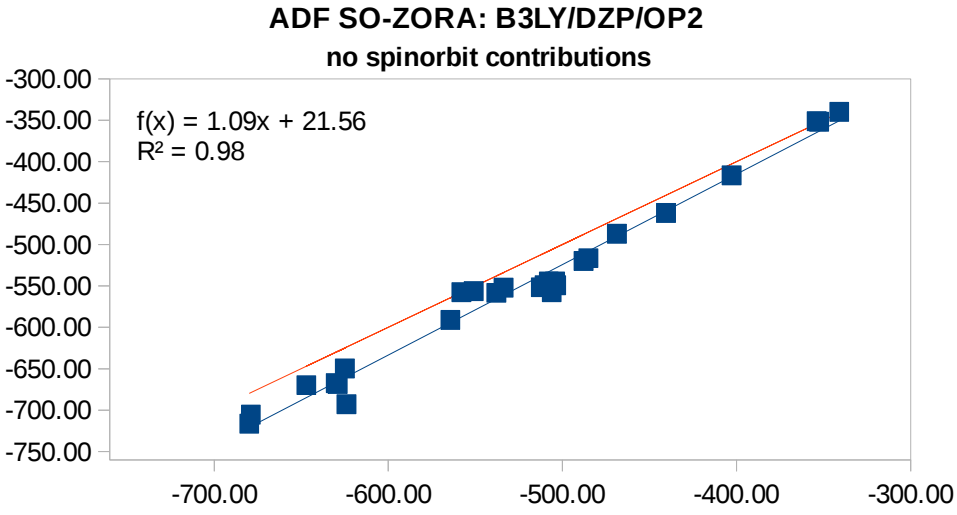


Table S32 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at SO [B3LYP/TZ2P)] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	δ(^{113}Cd)$_{fit}$ corrected by fit	ABS diff δ(^{113}Cd)$_{fit}$
1	-629.03	-729.99	101.0	-629.42	0.39
2	-624.03	-721.15	97.1	-621.08	2.95
3	-630.13	-729.68	99.5	-629.13	1.00
4	-624.93	-719.36	94.4	-619.40	5.53
5	-647.03	-733.54	86.5	-632.77	14.26
6	-506.13	-632.96	126.8	-537.89	31.76
7	-503.63	-617.09	113.5	-522.92	19.29
8	-512.33	-604.19	91.9	-510.75	1.58
9	-510.23	-607.20	97.0	-513.58	3.35
10	-487.83	-583.73	95.9	-491.44	3.61
11	-504.23	-620.38	116.2	-526.02	21.79
12	-507.83	-604.19	96.4	-510.75	2.92
13	-485.03	-579.69	94.7	-487.63	2.60
14	-352.53	-422.55	70.0	-339.39	13.14
15	-341.00	-410.38	69.4	-327.90	13.10
16	-354.00	-423.10	69.1	-339.91	14.09
17	-402.83	-486.16	83.3	-399.40	3.43
18	-440.46	-540.83	100.4	-450.97	10.51
19	-468.63	-569.72	101.1	-478.23	9.60
20	-537.93	-635.06	97.1	-539.87	1.94
21	-533.73	-628.56	94.8	-533.74	0.01
22	-550.93	-628.07	77.1	-533.27	17.66
23	-564.33	-662.50	98.2	-565.75	1.42
24	-558.03	-634.63	76.6	-539.46	18.57
25	-678.93	-775.03	96.1	-671.92	7.01
26	-679.83	-786.26	106.4	-682.51	2.68
		ME	126.83		
		MAE	94.25		
		CMAE	8.62		
		Slope	1.060		
		Int.	-62.80		

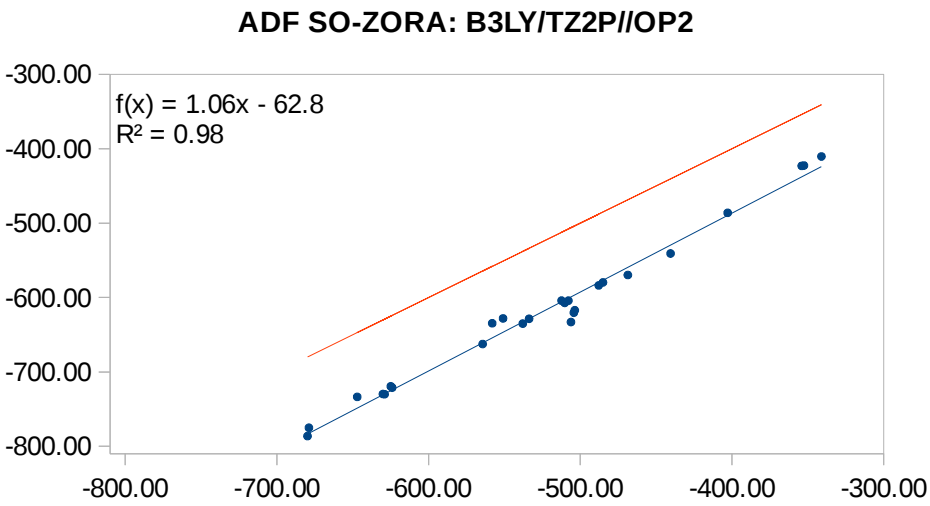


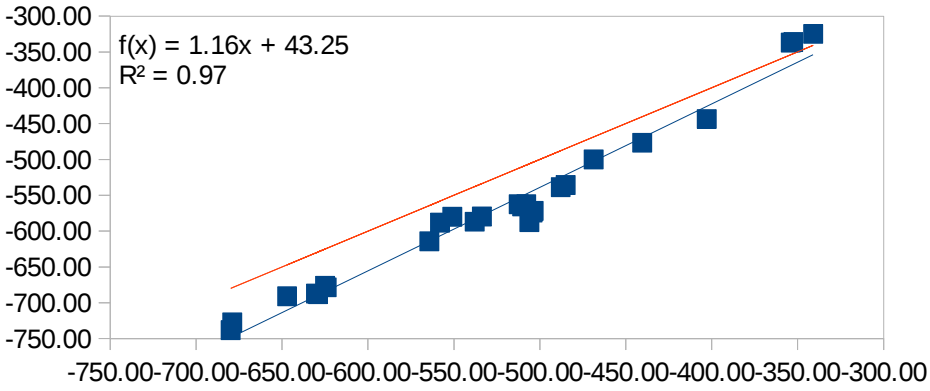
Table S33 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at SO [B3LYP/DZP)] level. Data are given without spin-orbit contributions. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	¡(^{113}Cd)$_{fit}$ corrected by fi	ABS diff δ(^{113}Cd)$_{fit}$
1	-629.03	-687.87	58.84	-628.11	7.94
2	-624.03	-678.36	54.33	-619.94	11.59
3	-630.13	-687.11	56.98	-627.46	9.73
4	-624.93	-676.36	51.43	-618.22	14.31
5	-647.03	-690.73	43.70	-630.57	23.33
6	-506.13	-587.26	81.13	-541.68	23.44
7	-503.63	-571.70	68.07	-528.31	11.78
8	-512.33	-562.49	50.16	-520.40	5.30
9	-510.23	-565.52	55.29	-523.00	0.45
10	-487.83	-538.76	50.93	-500.01	2.39
11	-504.23	-573.85	69.62	-530.15	13.13
12	-507.83	-562.49	54.66	-520.40	0.80
13	-485.03	-535.75	50.72	-497.42	2.34
14	-352.53	-336.32	16.21	-326.09	51.27
15	-341.00	-324.85	16.15	-316.23	50.18
16	-354.00	-336.91	17.09	-326.60	52.20
17	-402.83	-443.58	40.75	-418.24	3.99
18	-440.46	-476.63	36.17	-446.63	11.55
19	-468.63	-499.86	31.23	-466.59	18.59
20	-537.93	-586.87	48.94	-541.34	8.72
21	-533.73	-579.42	45.69	-534.94	11.30
22	-550.93	-579.93	29.00	-535.38	28.03
23	-564.33	-614.26	49.93	-564.87	10.21
24	-558.03	-588.17	30.14	-542.45	27.64
25	-678.93	-727.15	48.22	-661.86	22.10
26	-679.83	-737.90	58.07	-671.09	13.22

ME	81.13
MAE	46.67
CMAE	16.75
Slope	1.164
Int.	43.25

ADF SO-ZORA:B3LY/TZ2P//OP2

no spinorbit contributions



OP3 geometry [ADF relativistic scalar ZORA; B3LYP/TZ2P]

Table S34 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31G(d)] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	δ(^{113}Cd)$_{fit}$ corrected by fit	ABS diff δ(^{113}Cd)$_{fit}$
1	-629.03	-617.67	11.36	-616.78	12.25
2	-624.03	-638.91	14.88	-638.93	14.90
3	-630.13	-620.40	9.73	-619.63	10.50
4	-624.93	-623.06	1.87	-622.40	2.53
5	-647.03	-638.91	8.12	-638.93	8.10
6	-506.13	-540.59	34.46	-536.42	30.29
7	-503.63	-516.08	12.45	-510.87	7.24
8	-512.33	-512.92	0.59	-507.57	4.76
9	-510.23	-516.02	5.79	-510.81	0.58
10	-487.83	-484.76	3.07	-478.21	9.62
11	-504.23	-534.04	29.81	-529.59	25.36
12	-507.83	-510.25	2.42	-504.79	3.04
13	-485.03	-469.49	15.54	-462.30	22.73
14	-352.53	-359.87	7.34	-348.00	4.53
15	-341.00	-344.86	3.86	-332.35	8.65
16	-354.00	-353.95	0.05	-341.83	12.17
17	-402.83	-406.36	3.53	-396.47	6.36
18	-440.46	-449.47	9.01	-441.42	0.96
19	-468.63	-480.05	11.42	-473.30	4.67
20	-537.93	-561.12	23.19	-557.82	19.89
21	-533.73	-545.47	11.74	-541.51	7.78
22	-550.93	-564.85	13.92	-561.72	10.79
23	-564.33	-577.87	13.54	-575.28	10.95
24	-558.03	-556.27	1.76	-552.76	5.27
25	-678.93	-661.83	17.10	-662.83	16.10
26	-679.83	-670.30	9.53	-671.65	8.18

ME	34.46
MAE	10.62
CMAE	10.32
Slope	0.959
Int.	-26.09

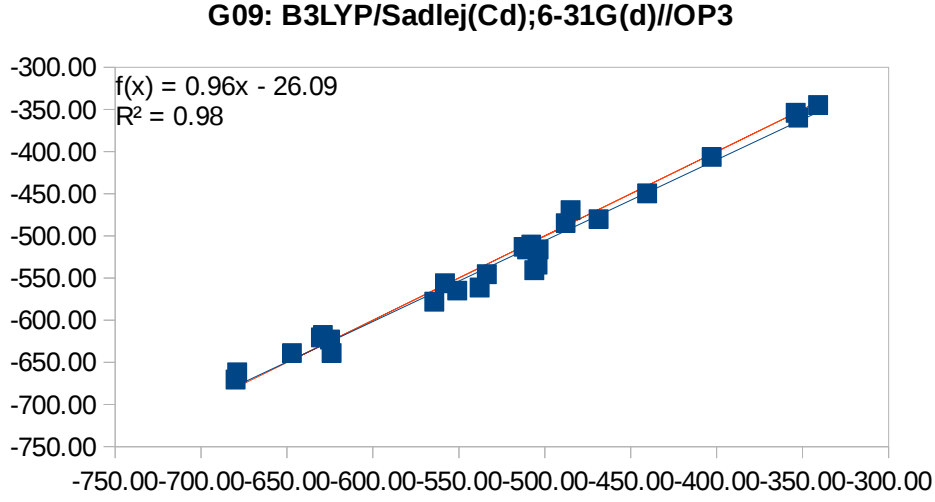


Table S35 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31G(d,p)] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	-629.03	-614.33	14.70	-619.04	9.99
2	-624.03	-610.93	13.10	-615.45	8.58
3	-630.13	-617.06	13.07	-621.92	8.21
4	-624.93	-619.69	5.24	-624.69	0.24
5	-647.03	-635.51	11.52	-641.41	5.62
6	-506.13	-536.82	30.69	-537.19	31.06
7	-503.63	-512.43	8.80	-511.42	7.79
8	-512.33	-509.73	2.60	-508.58	3.75
9	-510.23	-512.99	2.76	-512.01	1.78
10	-487.83	-481.91	5.92	-479.19	8.64
11	-504.23	-530.35	26.12	-530.34	26.11
12	-507.83	-507.19	0.64	-505.89	1.94
13	-485.03	-466.63	18.40	-463.05	21.98
14	-352.53	-357.02	4.49	-347.31	5.22
15	-341.00	-341.32	0.32	-330.72	10.28
16	-354.00	-351.44	2.56	-341.41	12.59
17	-402.83	-402.37	0.46	-395.19	7.64
18	-440.46	-446.06	5.60	-441.33	0.87
19	-468.63	-476.42	7.79	-473.40	4.77
20	-537.93	-557.26	19.33	-558.77	20.84
21	-533.73	-541.64	7.91	-542.27	8.54
22	-550.93	-560.90	9.97	-562.62	11.69
23	-564.33	-574.02	9.69	-576.47	12.14
24	-558.03	-551.88	6.15	-553.09	4.94
25	-678.93	-657.75	21.18	-664.89	14.04
26	-679.83	-666.41	13.42	-674.04	5.79

ME	30.69
MAE	10.09
CMAE	9.81
Slope	0.947
Int.	-28.15

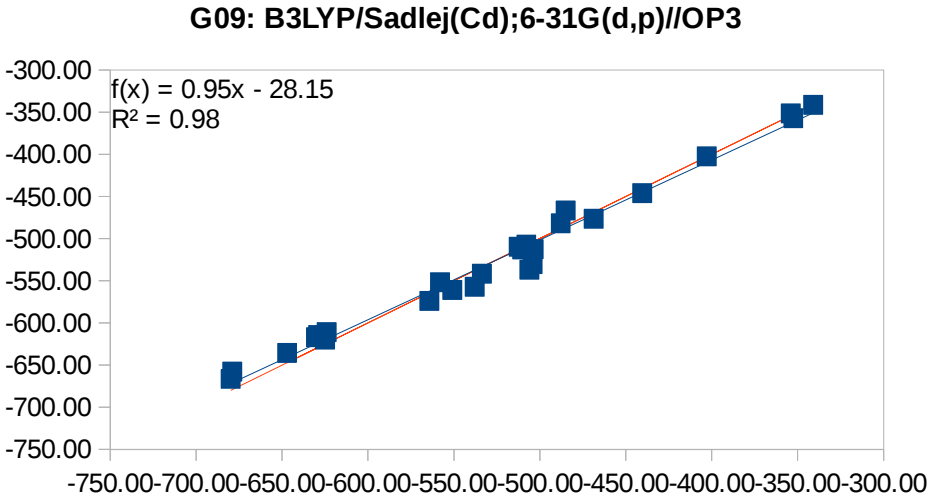


Table S36 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at NR-1 [B3LYP/Sadlej;6-31+G(d,p)] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	δ(^{113}Cd)$_{fit}$ corrected by fit	ABS diff δ(^{113}Cd)$_{fit}$
1	-629.03	-577.41	51.62	-614.35	14.68
2	-624.03	-580.92	43.11	-618.12	5.91
3	-630.13	-578.95	51.18	-616.01	14.12
4	-624.93	-582.11	42.82	-619.41	5.52
5	-647.03	-602.05	44.98	-640.85	6.18
6	-506.13	-506.38	0.25	-537.96	31.83
7	-503.63	-483.40	20.23	-513.26	9.63
8	-512.33	-478.43	33.90	-507.90	4.43
9	-510.23	-476.75	33.48	-506.10	4.13
10	-487.83	-450.23	37.60	-477.59	10.24
11	-504.23	-501.07	3.16	-532.26	28.03
12	-507.83	-478.81	29.02	-508.31	0.48
13	-485.03	-440.46	44.57	-467.08	17.95
14	-352.53	-332.81	19.72	-351.31	1.22
15	-341.00	-316.47	24.53	-333.74	7.26
16	-354.00	-326.49	27.51	-344.51	9.49
17	-402.83	-369.79	33.04	-391.08	11.75
18	-440.46	-415.12	25.34	-439.83	0.63
19	-468.63	-445.73	22.90	-472.74	4.11
20	-537.93	-526.71	11.22	-559.83	21.90
21	-533.73	-508.34	25.39	-540.08	6.35
22	-550.93	-527.10	23.83	-560.25	9.32
23	-564.33	-541.09	23.24	-575.29	10.96
24	-558.03	-520.04	37.99	-552.66	5.37
25	-678.93	-634.09	44.84	-675.30	3.63
26	-679.83	-640.89	38.94	-682.61	2.78
		ME	51.62		
		MAE	30.55		
		CMAE	9.54		
		Slope	0.930		
		Int.	-6.12		

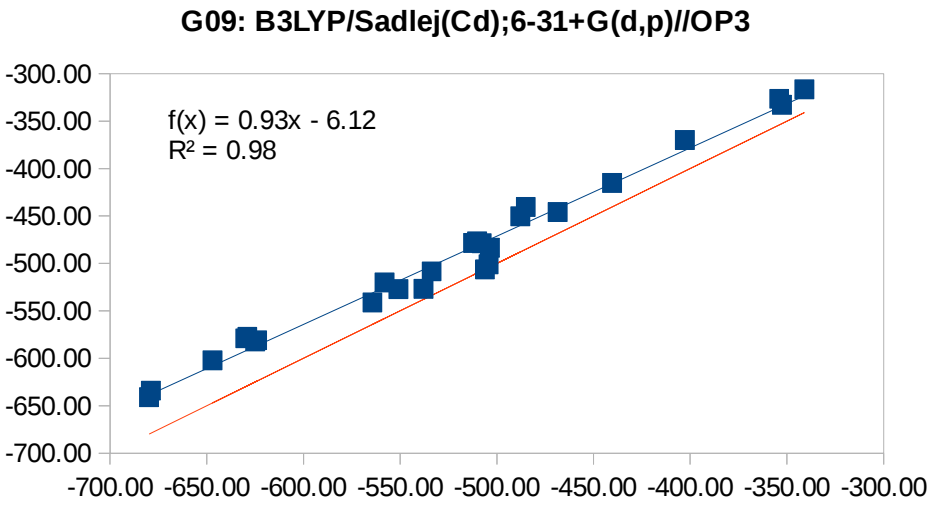


Table S37 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at NR-2 [B3LYP/DZP] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	-629.03	-678.59	49.56	-616.31	12.72
2	-624.03	-677.31	53.28	-615.03	9.00
3	-630.13	-680.18	50.05	-617.90	12.23
4	-624.93	-684.23	59.30	-621.94	2.99
5	-647.03	-702.13	55.10	-639.80	7.23
6	-506.13	-602.91	96.78	-540.78	34.65
7	-503.63	-578.04	74.41	-515.96	12.33
8	-512.33	-581.30	68.97	-519.22	6.89
9	-510.23	-586.45	76.22	-524.36	14.13
10	-487.83	-552.66	64.83	-490.63	2.80
11	-504.23	-596.59	92.36	-534.48	30.25
12	-507.83	-581.82	73.99	-519.73	11.90
13	-485.03	-538.22	53.19	-476.22	8.81
14	-352.53	-399.13	46.60	-337.41	15.12
15	-341.00	-383.12	42.12	-321.43	19.57
16	-354.00	-395.51	41.51	-333.80	20.20
17	-402.83	-451.46	48.63	-389.63	13.20
18	-440.46	-509.36	68.90	-447.42	6.96
19	-468.63	-529.69	61.06	-467.71	0.92
20	-537.93	-616.60	78.67	-554.45	16.52
21	-533.73	-602.43	68.70	-540.30	6.57
22	-550.93	-622.83	71.90	-560.66	9.73
23	-564.33	-640.26	75.93	-578.06	13.73
24	-558.03	-607.55	49.52	-545.41	12.62
25	-678.93	-721.43	42.50	-659.07	19.86
26	-679.83	-730.27	50.44	-667.89	11.94
		ME	96.78		
		MAE	62.10		
		CMAE	12.80		
		Slope	1.002		
		Int.	-61.05		

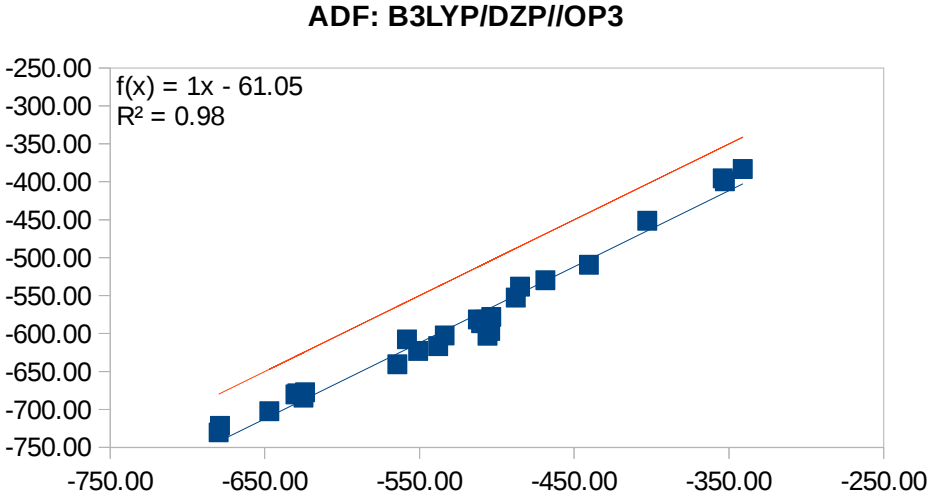


Table S38 Calculated $\delta(^{113}Cd)$, statistical data and graphical correlation obtained at NR-2 [B3LYP/TZ2P] level. Data referred wrt Me_2Cd.

MODEL	Exptl.$\delta(^{113}Cd)$	Calcd $\delta(^{113}Cd)$	ABS diff $\delta(^{113}Cd)$	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	-629.03	-667.78	38.75	-614.83	15.35
2	-624.03	-664.18	40.15	-611.37	13.82
3	-630.13	-669.38	39.25	-616.37	14.92
4	-624.93	-671.81	46.88	-618.71	7.38
5	-647.03	-688.72	41.69	-634.97	13.22
6	-506.13	-600.28	94.15	-549.93	42.64
7	-503.63	-571.11	67.48	-521.88	17.09
8	-512.33	-572.66	60.33	-523.37	9.88
9	-510.23	-576.24	66.01	-526.81	15.43
10	-487.83	-536.72	48.89	-488.81	0.17
11	-504.23	-589.01	84.78	-539.09	33.71
12	-507.83	-573.02	65.19	-523.72	14.73
13	-485.03	-525.16	40.13	-477.70	8.49
14	-352.53	-379.07	26.54	-337.23	16.46
15	-341.00	-359.91	18.91	-318.80	23.35
16	-354.00	-374.86	20.86	-333.18	21.98
17	-402.83	-433.76	30.93	-389.81	14.17
18	-440.46	-486.56	46.1	-440.58	1.03
19	-468.63	-511.65	43.02	-464.71	5.08
20	-537.93	-599.23	61.3	-548.92	9.83
21	-533.73	-588.37	54.64	-538.48	3.59
22	-550.93	-608.14	57.21	-557.48	5.40
23	-564.33	-624.47	60.14	-573.19	7.70
24	-558.03	-600.32	42.29	-549.97	9.22
25	-678.93	-718.86	39.93	-663.95	16.14
26	-679.83	-724.34	44.51	-669.22	11.77
		ME	94.15		
		MAE	49.23		
		CMAE	13.56		
		Slope	1.040		
		Int.	-28.36		

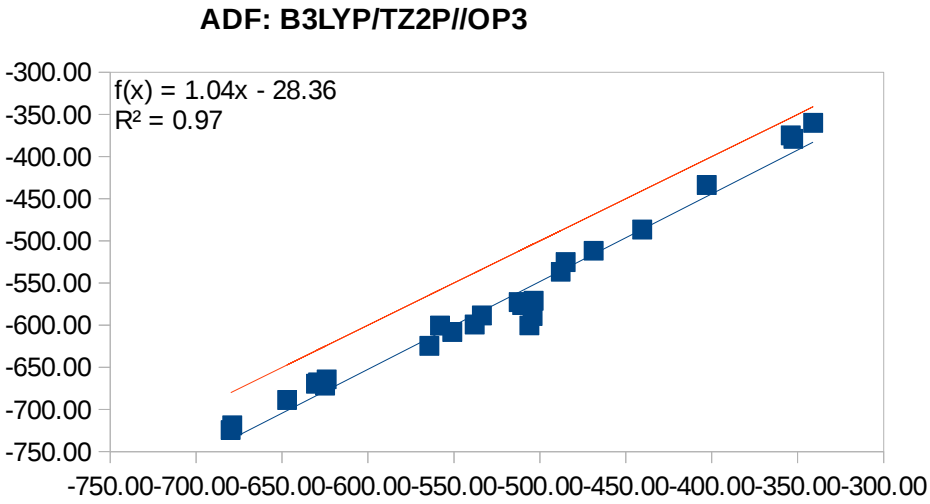


Table S39 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at SR [B3LYP/DZP] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	-629.03	-614.07	14.96	-614.82	14.21
2	-624.03	-638.22	14.19	-637.34	13.31
3	-630.13	-612.98	17.15	-613.80	16.33
4	-624.93	-594.93	30.00	-596.96	27.97
5	-647.03	-615.75	31.28	-616.38	30.65
6	-506.13	-502.92	3.21	-511.14	5.01
7	-503.63	-492.36	11.27	-501.29	2.34
8	-512.33	-496.41	15.92	-505.06	7.27
9	-510.23	-493.88	16.35	-502.70	7.53
10	-487.83	-464.57	23.26	-475.37	12.46
11	-504.23	-490.35	13.88	-499.41	4.82
12	-507.83	-489.53	18.30	-498.65	9.18
13	-485.03	-461.20	23.83	-472.22	12.81
14	-352.53	-301.46	51.07	-323.22	29.31
15	-341.00	-289.72	51.28	-312.27	28.73
16	-354.00	-300.48	53.52	-322.30	31.70
17	-402.83	-402.40	0.43	-417.37	14.54
18	-440.46	-456.79	16.33	-468.11	27.65
19	-468.63	-485.12	16.49	-494.53	25.90
20	-537.93	-577.33	39.40	-580.55	42.62
21	-533.73	-569.19	35.46	-572.95	39.22
22	-550.93	-592.67	41.74	-594.85	43.92
23	-564.33	-609.87	45.54	-610.90	46.57
24	-558.03	-583.39	25.36	-586.20	28.17
25	-678.93	-650.12	28.81	-648.44	30.49
26	-679.83	-661.13	18.70	-658.71	21.12

ME	53.52
MAE	25.30
CMAE	22.07
Slope	1.072
Int.	45.05

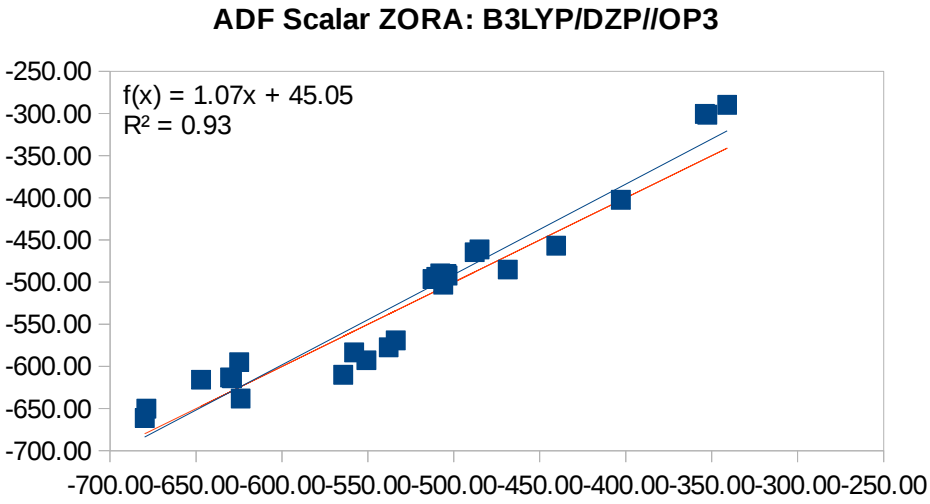


Table S40 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at SR [B3LYP/TZ2P] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	δ(^{113}Cd)$_{fit}$ corrected by fit	ABS diff δ(^{113}Cd)$_{fit}$
1	-629.03	-652.69	23.66	-608.53	20.50
2	-624.03	-652.61	28.58	-608.46	15.57
3	-630.13	-655.15	25.02	-610.67	19.46
4	-624.93	-658.99	34.06	-614.02	10.91
5	-647.03	-676.85	29.82	-629.57	17.46
6	-506.13	-590.42	84.29	-554.31	48.18
7	-503.63	-562.84	59.21	-530.30	26.67
8	-512.33	-554.97	42.64	-523.44	11.11
9	-510.23	-557.93	47.70	-526.02	15.79
10	-487.83	-523.42	35.59	-495.97	8.14
11	-504.23	-582.07	77.84	-547.04	42.81
12	-507.83	-554.28	46.45	-522.84	15.01
13	-485.03	-509.04	24.01	-483.45	1.58
14	-352.53	-321.17	31.36	-319.86	32.67
15	-341.00	-304.74	36.26	-305.56	35.44
16	-354.00	-318.11	35.89	-317.20	36.80
17	-402.83	-421.85	19.02	-407.53	4.70
18	-440.46	-464.44	23.98	-444.62	4.16
19	-468.63	-490.90	22.27	-467.66	0.97
20	-537.93	-594.90	56.97	-558.21	20.28
21	-533.73	-578.69	44.96	-544.10	10.37
22	-550.93	-602.17	51.24	-564.54	13.61
23	-564.33	-619.37	55.04	-579.52	15.19
24	-558.03	-592.89	34.86	-556.46	1.57
25	-678.93	-704.47	25.54	-653.62	25.31
26	-679.83	-714.16	34.33	-662.06	17.77
		ME	84.29		
		MAE	39.64		
		CMAE	18.16		
		Slope	1.148		
		Int.	46.18		

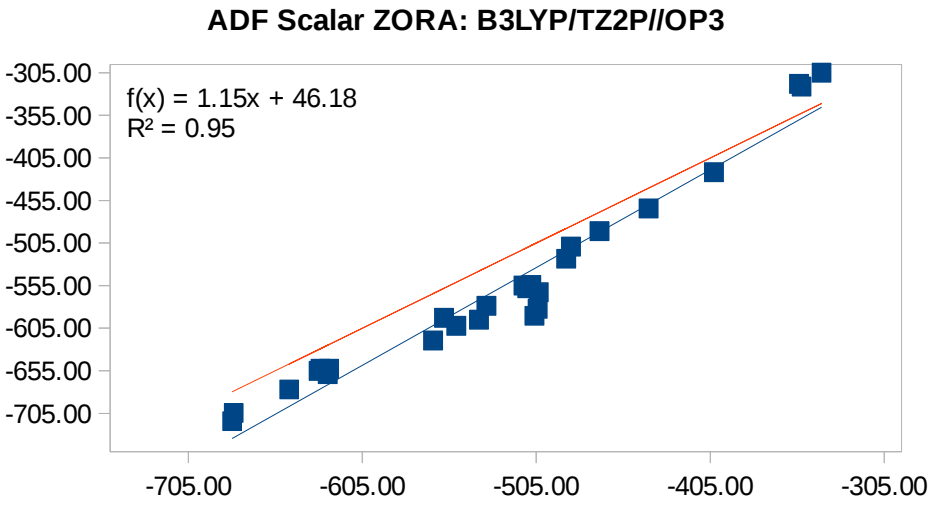


Table S41 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at SO [B3LYP/DZP] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	-629.03	-671.22	42.19	-612.67	16.36
2	-624.03	-678.84	54.81	-620.65	3.38
3	-630.13	-674.48	44.35	-616.09	14.04
4	-624.93	-677.41	52.48	-619.15	5.78
5	-647.03	-694.99	47.96	-637.56	9.47
6	-506.13	-609.74	103.61	-548.31	42.18
7	-503.63	-581.49	77.86	-518.74	15.11
8	-512.33	-575.81	63.48	-512.79	0.46
9	-510.23	-578.63	68.40	-515.74	5.51
10	-487.83	-544.56	56.73	-480.07	7.76
11	-504.23	-601.80	97.57	-540.00	35.77
12	-507.83	-572.92	65.09	-509.76	1.93
13	-485.03	-528.80	43.77	-463.58	21.45
14	-352.53	-423.73	71.20	-353.58	1.05
15	-341.00	-405.13	64.13	-334.11	6.89
16	-354.00	-419.43	65.43	-349.08	4.92
17	-402.83	-430.31	27.48	-360.47	42.36
18	-440.46	-509.83	69.37	-443.72	3.26
19	-468.63	-548.04	79.41	-483.72	15.09
20	-537.93	-609.97	72.04	-548.55	10.62
21	-533.73	-592.86	59.13	-530.64	3.09
22	-550.93	-619.52	68.59	-558.55	7.62
23	-564.33	-638.58	74.25	-578.50	14.17
24	-558.03	-604.09	46.06	-542.40	15.63
25	-678.93	-729.97	51.04	-674.18	4.75
26	-679.83	-738.35	58.52	-682.95	3.12

ME	103.61
MAE	62.50
CMAE	11.99
Slope	0.955
Int.	-85.99

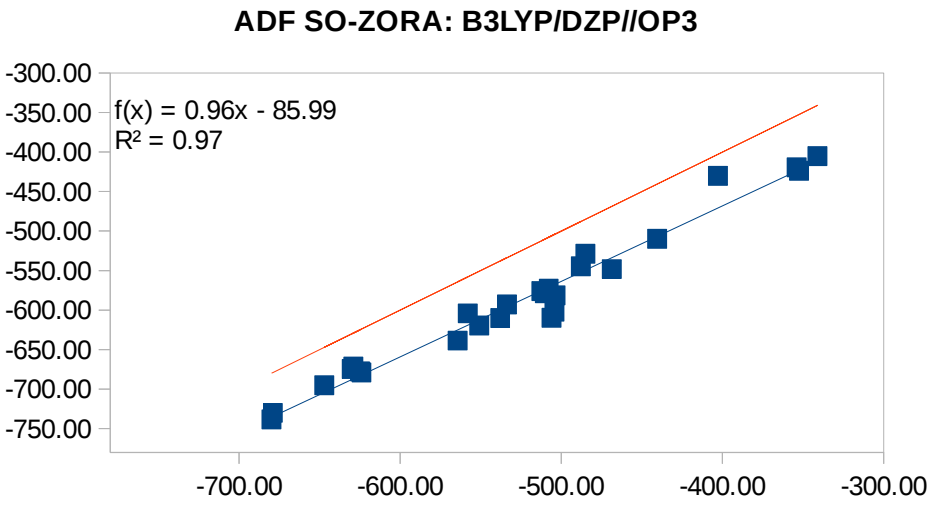


Table S42 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at SO [B3LYP/DZP)] level. Data are given without spin-orbit contributions. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	δ(^{113}Cd)$_{fit}$ corrected by fit	ABS diff δ(^{113}Cd)$_{fit}$
1	-629.03	-641.21	12.18	-611.19	17.84
2	-624.03	-646.22	22.19	-615.78	8.25
3	-630.13	-644.40	14.26	-614.11	16.02
4	-624.93	-647.10	22.17	-616.59	8.34
5	-647.03	-664.79	17.76	-632.84	14.19
6	-506.13	-576.49	70.36	-551.76	45.63
7	-503.63	-548.27	44.64	-525.85	22.22
8	-512.33	-542.98	30.65	-520.99	8.66
9	-510.23	-548.60	38.37	-526.15	15.92
10	-487.83	-513.58	25.74	-493.98	6.15
11	-504.23	-568.62	64.39	-544.53	40.30
12	-507.83	-543.09	35.26	-521.09	13.26
13	-485.03	-497.94	12.91	-479.62	5.41
14	-352.53	-336.11	16.42	-331.02	21.51
15	-341.00	-319.63	21.37	-315.89	25.11
16	-354.00	-332.33	21.67	-327.55	26.45
17	-402.83	-403.63	0.80	-393.02	9.81
18	-440.46	-456.40	15.94	-441.48	1.02
19	-468.63	-485.67	17.04	-468.36	0.27
20	-537.93	-579.20	41.27	-554.24	16.31
21	-533.73	-560.32	26.58	-536.90	3.17
22	-550.93	-586.20	35.27	-560.68	9.75
23	-564.33	-605.87	41.54	-578.74	14.41
24	-558.03	-571.03	13.00	-546.74	11.29
25	-678.93	-693.73	14.80	-659.41	19.52
26	-679.83	-702.02	22.19	-667.03	12.80
		ME	70.36		
		MAE	26.88		
		CMAE	15.14		
		Slope	1.089		
		Int.	24.37		

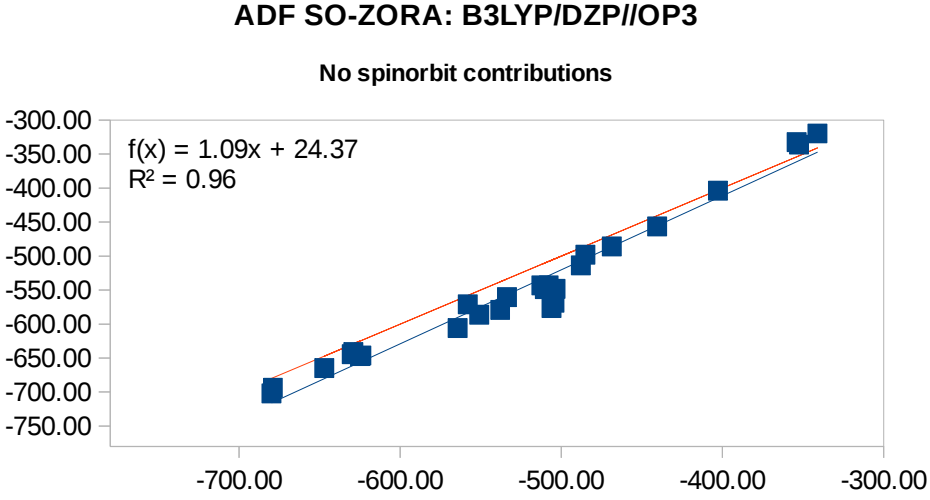


Table S43 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at SO [B3LYP/TZ2P] level. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	-629.03	-696.75	67.72	-607.76	21.27
2	-624.03	-698.44	74.41	-609.37	14.66
3	-630.13	-699.45	69.32	-610.33	19.80
4	-624.93	-703.85	78.92	-614.53	10.40
5	-647.03	-722.44	75.41	-632.25	14.78
6	-506.13	-638.20	132.07	-551.94	45.81
7	-503.63	-612.68	109.05	-527.62	23.99
8	-512.33	-601.31	88.98	-516.78	4.45
9	-510.23	-601.59	91.36	-517.04	6.81
10	-487.83	-571.49	83.66	-488.35	0.52
11	-504.23	-631.82	127.59	-545.86	41.63
12	-507.83	-597.85	90.02	-513.48	5.65
13	-485.03	-555.91	70.88	-473.50	11.53
14	-352.53	-405.46	52.93	-330.08	22.45
15	-341.00	-388.31	47.31	-313.72	27.28
16	-354.00	-399.30	45.30	-324.20	29.80
17	-402.83	-468.24	65.41	-389.92	12.91
18	-440.46	-531.06	90.60	-449.81	9.35
19	-468.63	-563.27	94.64	-480.51	11.88
20	-537.93	-644.39	106.46	-557.85	19.92
21	-533.73	-630.25	96.52	-544.37	10.64
22	-550.93	-654.47	103.54	-567.45	16.52
23	-564.33	-670.52	106.19	-582.76	18.43
24	-558.03	-643.42	85.39	-556.92	1.11
25	-678.93	-752.04	73.11	-660.47	18.46
26	-679.83	-757.95	78.12	-666.10	13.73

ME	132.07
MAE	84.80
CMAE	16.68
Slope	1.049
Int.	-59.21

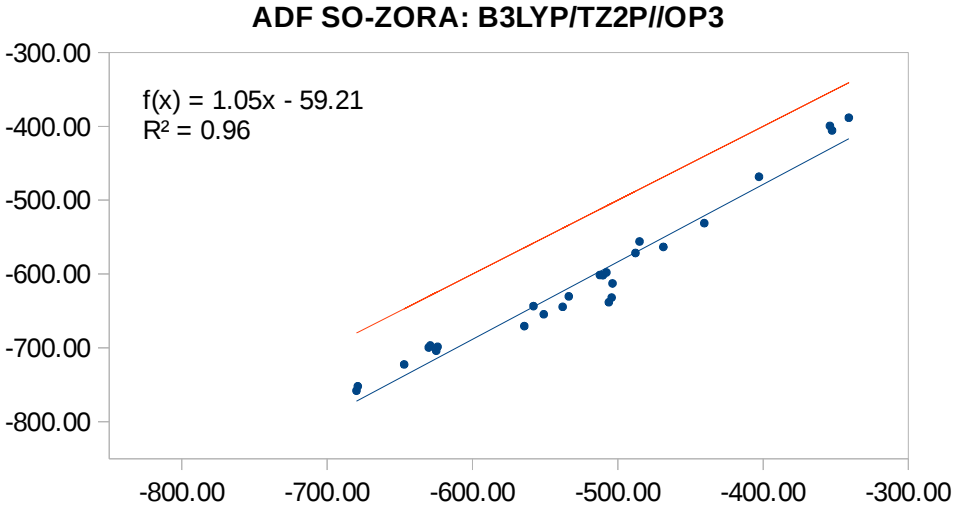


Table S44 Calculated δ(^{113}Cd), statistical data and graphical correlation obtained at SO [B3LYP/TZ2P)] level. Data are given without spin-orbit contributions. Data referred wrt Me_2Cd.

MODEL	Exptl.δ(^{113}Cd)	Calcd δ(^{113}Cd)	ABS diff δ(^{113}Cd)	$\delta(^{113}Cd)_{fit}$ corrected by fit	ABS diff $\delta(^{113}Cd)_{fit}$
1	-629.03	-657.66	28.63	-613.31	28.38
2	-624.03	-658.16	34.13	-613.74	22.96
3	-630.13	-660.21	30.07	-615.51	27.31
4	-624.93	-664.25	39.32	-619.01	18.65
5	-647.03	-682.21	35.18	-634.58	25.39
6	-506.13	-596.82	90.69	-560.58	42.50
7	-503.63	-569.82	66.19	-537.19	21.92
8	-512.33	-560.21	47.88	-528.86	5.00
9	-510.23	-563.07	52.84	-531.34	9.55
10	-487.83	-529.84	42.01	-502.54	3.54
11	-504.23	-589.09	84.86	-553.89	37.80
12	-507.83	-559.37	51.54	-528.14	8.79
13	-485.03	-515.09	30.06	-489.76	6.27
14	-352.53	-318.31	34.22	-319.24	42.00
15	-341.00	-303.48	37.52	-306.39	43.15
16	-354.00	-312.08	41.92	-313.84	48.80
17	-402.83	-415.34	12.51	-403.32	9.35
18	-440.46	-468.21	27.75	-449.14	1.78
19	-468.63	-494.43	25.80	-471.86	7.53
20	-537.93	-563.04	25.11	-531.31	18.18
21	-533.73	-547.90	14.17	-518.19	26.92
22	-550.93	-571.12	20.19	-538.31	24.27
23	-564.33	-625.99	61.66	-585.86	9.24
24	-558.03	-598.83	40.80	-562.33	7.68
25	-678.93	-709.03	30.10	-657.82	34.36
26	-679.83	-701.01	21.18	-650.87	42.13
		ME	90.69		
		MAE	39.47		
		CMAE	22.06		
		Slope	1.154		
		Int.	50.10